

NLTE Line Formation Calculations
for Hydrogen and Ionized Helium
in Photospheres of Very Hot Stars

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**NLTE Line Formation Calculations
for Hydrogen and Ionized Helium
in Photospheres of Very Hot Stars**

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ABSTRACT

In this work we apply the recently developed technique of the Accelerated Lambda Iteration to Hydrogen and Helium II line formation problems in very hot stars with $T_{\text{eff}} \geq 30000$ K.

First, treating Hydrogen and Helium separately, we investigate the effect of including more levels and Stark broadening in the statistical equilibrium equations. Then we treat for the first time the problem of the full overlap of Hydrogen and Helium lines.

Our results may be summarised as follows:

- A Hydrogen model atom must include 10 NLTE levels with all the bound - bound transitions coupling them and Stark broadening for the lines with upper level $n \leq 7$ to achieve an accuracy better than present day observations.

- The new calculations for Hydrogen resolve the discrepancy between older calculations and the observed profiles in the cores of the Balmer profiles of slowly rotating stars.

- The HeII atom should contain 14 NLTE levels with all the bound - bound transitions coupling them and Stark broadening for the lines with upper level $n \leq 7$.

- The resonance lines of HeII may be treated in detailed balancing when $T_{\text{eff}} \leq 75000$ K. In addition the ground level continuum of HeII may be so treated when $T_{\text{eff}} \leq 50000$ K for extreme Helium rich models or when $T_{\text{eff}} \leq 38000$ K for normal Helium abundances.

- The new profiles may be of special importance for the quantitative analysis of CPN.

- The overlap of the H and HeII lines has no influence on the visible lines of these two elements. Therefore, they can be treated separately.

CHAPTER I

Introduction

The very hot stars, with temperatures in excess of 30000 K, constitute a very inhomogenous group. They are found as young and luminous stars or as old, highly evolved subluminous objects; as very massive stars with strong winds or as small and compact ones; in globular cluster, in the halo or in the disk. In all cases, they have strong UV fluxes (which sometimes makes the optical observations difficult) and are recognized by their very blue colours. The accurate placement of all these objects in the HR diagram is the first step to their interpretation. However, their analysis is extremely difficult. The strong radiation field produces very large radiative rates in their photospheres overcoming the electron collision rates and coupling it to the atomic populations. The consequence is a breakdown of the LTE (*Peterson and Scholz*, 1971). The high temperatures on the other hand prevent the use of continuum methods. This was convincingly demonstrated by *Kudritzki et al.* (1983) in their analysis of ζ Puppis, in which they showed that temperature and gravity must be determined simultaneously. A recent analysis of the inadequacy of continuum methods has been given by *Abbott and Hummer* (1985).

Thus a careful determination of these stellar parameters (including also the abundances) requires the elaborate NLTE theory of radiative transfer, developed by *Auer and Mihalas* (1969). The first detailed calculations and analyses were carried out by the same authors (*Auer and Mihalas*, 1972). In the years following, an extensive application of these techniques, together with an improvement in the quality of the observational data, allowed more information to be obtained about the physical conditions that dominate in these stars.

Unfortunately, quantitative spectroscopy could until now only be made with photospherical absorption lines. Phenomena such as sphericity effects, extended envelopes, stellar winds and mass loss, which produce emission lines and P - Cygni profiles, are not treated with sufficient accuracy by present theories and computer facilities. For this reason, we describe here only those groups of stars that allow such a spectroscopic analysis (although they may show other characteristics too).

Thus, we wish to summarise our present knowledge about the photospheres of the very hot stars and to emphasize the importance of an accurate determination of the basic stellar parameters: temperature, gravity, abundances. We start by giving an overview of the hot stars and discuss then each group separately.

1.1. – The Hot Stars in the HR Diagram

The positions of the very hot stars in the $\log g - \log T_{\text{eff}}$ diagram are displayed in Fig 1.2. For comparison, the same regions are plotted in the usual $\log L - \log T_{\text{eff}}$ representation in Fig 1.1. The advantage of the first diagram is that both parameters, g and T_{eff} , may be determined directly from the observed spectra, so that stars can be represented in the diagram without knowledge of their luminosities or distances (see *Newell, 1973*).

It can be seen from the figures that the very hot stars actually cover a wide range of temperatures and gravities. We distinguish three groups: the massive O stars, the subluminous OB stars and the Central Stars of Planetary Nebulae (CPN).

The O stars are highly luminous and hence very massive objects. Because such objects will consume their nuclear combustible material very rapidly they must be young stars. In fact, as can be seen in the figures their gravities are usually slightly lower than those of ZAMS stars, indicating extended envelopes and evolution.

Therefore, O stars are strongly coupled to the physics of stellar formation and to the energy balance of the interstellar medium, to which they release the energy of their supersonic stellar winds. They allow a detailed study of the conditions in other galaxies because of their high luminosities. Finally, they explode as type II supernovae at the end of their lives.

The other two groups are compact subluminous objects. At these temperatures, this means small radius and low masses. They are then highly evolved objects, whose evolutionary status lies between the giant and the white dwarf stages. Thus, they are of crucial importance in our understanding of the evolution of low and intermediate mass stars. Clearly, CPN are also strongly related with the interstellar medium and its chemical evolution.

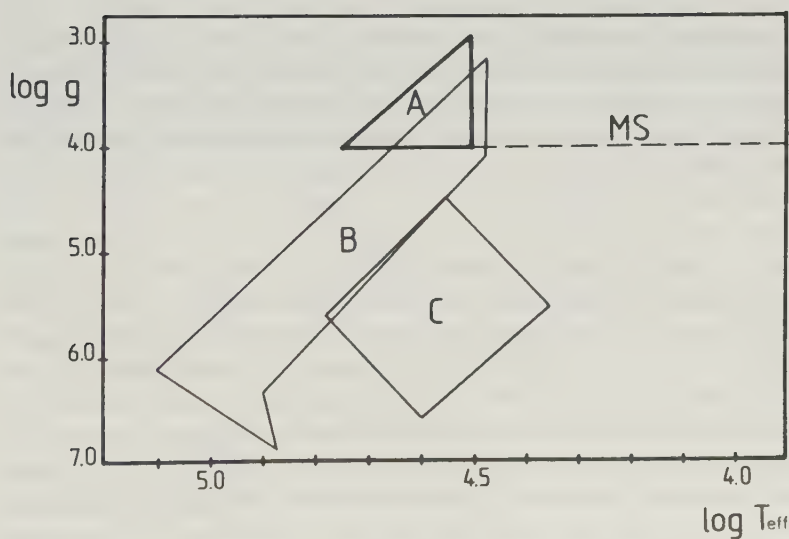
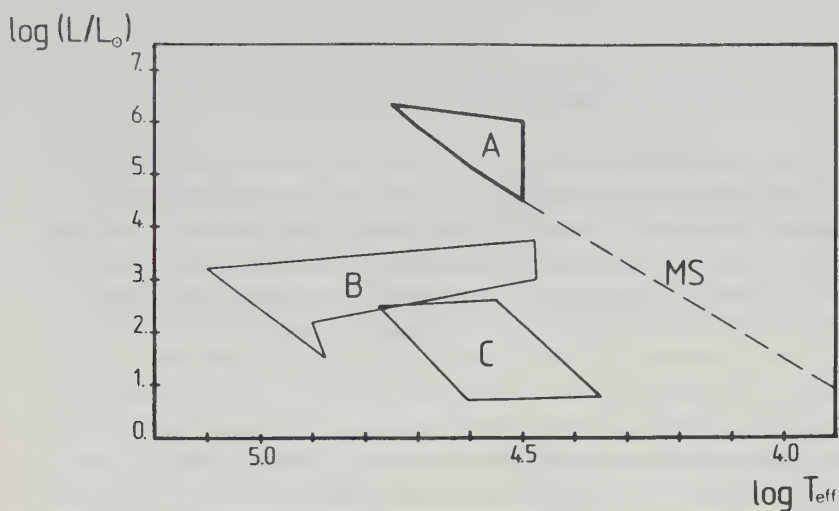


Fig. 1.1 (upper) and 1.2 (lower): The position of the O and Of stars (A), the CPN (B) and the sdO and sdB (C) in the usual $\log L - \log T_{\text{eff}}$ diagram and in the $\log g - \log T_{\text{eff}}$ representation.

1.2. – The Massive O and Of Stars

The most massive stars in the main sequence are divided into O and Of stars. They are distinguished by their spectra: O types present a normal absorption line spectrum, whereas Of (a subgroup of the O stars) show emission lines of NIII ($\lambda\lambda 4634 - 40 - 41$) and HeII ($\lambda 4686$) together with absorption lines of the same ions. This means that a selective mechanism is needed to produce the emission.

After a qualitative analysis of their spectra *Walborn* (1970, 1971, 1982) divided the Of stars into several groups: Of* (for the most extreme ones), Of, O(f) and O((f)). During the same work *Walborn* (1971) found that some OB stars show strong nitrogen lines (OBN stars) or strong carbon lines (OBC). Moreover, carbon enhancement was usually accompanied by nitrogen deficiency and vice versa. This resembles the WN/WC dichotomy found in Wolf – Rayet stars.

Conti and Alschuler (1971) investigated the spectra of hot stars and established a spectral classification based on the ratio HeI 4471/HeII 4541, which constitutes a temperature criterium. As luminosity indicator they used the ratio SiIV 4089/HeI 4143, but it is not very sensitive. They concluded that Of stars are more luminous and massive than O stars.

As already mentioned above, the quantitative spectroscopy of O stars began with the work of *Auer and Mihalas* (1972). They constructed NLTE models running from $T_{\text{eff}} = 30000$ to 50000 K and $\log g = 3.3$ to 4.5 , and applied them to 10 O stars. This work showed that the NLTE theory reproduces the observed line profiles much better than the LTE one, although the computed Balmer profiles were usually too shallow when the adopted rotational velocity was small. In addition they tried to obtain the HeII $\lambda 4686$ emission by pumping the $2 \leftrightarrow 4$ transition of HeII by $L_{\gamma} - \alpha$ (the so called "Bowen mechanism", *Bowen*, 1935). They investigated two limiting cases to estimate the effect of this pumping: no overlap of Hydrogen and Helium lines and exact coincidence of the appropriate lines. Although they could not clearly distinguish between the two cases in their analysis of the observations, they indicated that neutralization of the line was the best they could obtain. Moreover, *Mihalas and Lockwood* (1972) showed that the full overlap of Hydrogen and Helium lines produces much too large equivalent widths in the $4 \leftrightarrow 5$ transition of HeII at $\lambda 10124$, in contrast to the non – overlap case, which produces qualitatively better agreement with the observations. Howe-

ver, the actual effect when the overlap is treated correctly remains unknown.

The effect of an extended atmosphere, often proposed as an explanation of this HeII $\lambda 4686$ emission in Of stars, was investigated by *Kunasz et al.* (1975), who constructed a grid of spherical models and showed that it is possible to bring the line selectively into emission due to atmospheric extension. Nevertheless, as pointed out by these authors, in such atmospheres dynamical effects are very important, so that their static models only give qualitative agreement with the observations of Of stars.

The NIII emission at $\lambda\lambda 4634, 4640, 4641$ is present not only in the Of types, but also in the O(f) and O((f)) stars. These last types have compact atmospheres, so that the explanation of this effect must be qualitatively different from that of the HeII $\lambda 4686$ emission. In fact, as showed by *Mihalas and Hummer* (1973), the emission in O(f) and O((f)) stars is a consequence of the atomic structure and processes of NIII: the upper states of the multiplet are overpopulated due to dielectronic recombination from an autoionizing state. Electrons cascade then to the lower levels of the multiplet. At the same time, these levels produce no emission lines at $\lambda\lambda 4097, 4013$ by further cascades, due to two electron transitions. Of stars are actually not considered, because the authors used static plane - parallel models. This work shows clearly how important is a correct description of the atomic models.

Using the spectral classification of *Conti and Alschuler* (1971) and the models of *Auer and Mihalas* (1972), *Conti* (1973a,b) constructed a spectroscopic temperature scale. He showed that main sequence stars have gravities of about 4.0 and supergiants of about 3.3. However, the line ratio HeI $4471/\text{HeII } 4541$ used to derive the spectral type is gravity dependent, so that Conti in fact derived two scales, one for main sequence stars ranging from 33000 K (O9.5) to 50000 K (O4) and one for supergiants, about ten percent cooler. More recently *Conti and Frost* (1977) extended the scale to type O3 (55000 K).

Kudritzki (1980), *Simon et al.* (1983) and *Kudritzki et al.* (1983) performed detailed quantitative spectroscopic analyses of early O stars. They concluded that these stars are cooler than assumed by Conti and Frost. The explanation is that their gravities are lower than 4.0, the value assigned by Conti and Frost to the main sequence, because all them are more or less evolved. A classic example of this

effect is found for the star ζ Pup (O4f). From angular diameter and energy distribution, a temperature around 35000 K is deduced (see, for example, *Remie and Lamers*, 1981). From the temperature scale of Conti and Frost, however, the temperature is 50000 K.

This is a clear contradiction. The solution, as shown by *Kudritzki et al.* (1983), is that the gravity dependence was not taken into account. When this is made, a spectroscopic temperature of 42000 K and a $\log g$ of 3.5 are obtained together with a continuum energy distribution that fits the observed one. This work shows that for very hot stars only detailed quantitative spectroscopy is accurate enough to give the correct stellar parameters, owing to the interdependence of temperature, gravity and abundances.

In the papers cited above it can be seen that the Of stars are more evolved than the O stars. A scenario in which O stars evolve through mass loss into Of stars and then into WR stars was proposed by *Conti* (1975). This was studied by *Noels and Gabriel* (1981) and *Maeder* (1981), who found that the mass loss rates needed to expose the processed material of the inner layers (mixed by convection) were larger than observed. The problem was solved by introducing convective overshooting into the theoretical evolutionary models (*Bressan et al.*, 1981; *Doom*, 1982a,b; *Maeder*, 1982). The new convective cores were now larger and smaller mass loss rates were necessary. Thus, very massive stars ($M \geq 50M_{\odot}$, *Maeder*, 1982; $M \geq 33M_{\odot}$, *Doom*, 1982a,b) follow *Conti's* scenario, whereas less massive stars ($M \geq 20M_{\odot}$) evolve into the WR phase only after passing through the Of and Red Supergiant stage (*Maeder*, 1982; *Doom et al.*, 1986). The masses separating both scenarios agree qualitatively with estimates based on observations, but they do not allow the two scenarios to be distinguished: *Bertelli et al.* (1984) give 30 – 40 $M_{\odot}$, *Conti et al.* (1983) 40 $M_{\odot}$ and *Humphreys et al.* (1985) 50 $M_{\odot}$. Other mechanisms, such as binarity, can also contribute to Of formation.

When the stars reach the Of stage, CNO processed material appears discontinuously at their surfaces (*Maeder*, 1985; *Prantzos et al.*, 1986). N and He are enriched, whereas the C and O abundances decrease. The study of the abundances at the surface of the stars supplies then indications about its evolutionary status and at the same time, is an important test of the theoretical evolutionary scenarios.

Unfortunately, the study of the abundances in very hot stars is enormously complicated by effects like NLTE. The results obtained by the detailed spectroscopic analyses of Kudritzki, Kudritzki et al. and Simon et al. cited above indicate only that ζ Puppis – the most evolved star studied there – shows a slightly enhanced content of Helium, whereas all other stars have normal Helium abundances. A more recent work (*Butler and Simon*, 1985) shows that ζ Pup has an increased nitrogen abundance. Although all these facts agree with the current evolutionary theories, only a total of five objects were analyzed in these papers. Clearly, a greater number of detailed analyses is required.

Some of the Of stars are also OBN stars. The evolutionary status of some of these stars is still unclear. The recent work of *Schönberner et al.* (1986) shows not only that they are nitrogen rich and carbon poor, as inspection of their spectra indicate, but also that Helium is enriched in the atmospheres of these stars. Both facts together point to processed CNO material in the atmosphere, which agrees with the expectations in those OBN stars showing Of characteristics (or being clearly away from the ZAMS). However the abundances are quantitatively not in agreement with evolutionary calculations and two of the four OBN objects of Schönberner et al. lie close to the ZAMS (*Kudritzki*, 1985). Very recently *Maeder* (1986) included turbulent diffusion induced by rotation in his calculations. A star then remains near the ZAMS as it evolves, and mixing is produced at the beginning of the MS evolution, with CNO and He abundance values that agree more closely with the ones derived by Schönberner et al. This scenario is only possible if the star has a very high rotational velocity, so that OBN stars should be very fast rotators. Maeder estimates from observations $v \sin i \geq 350$ km/s. However the objects of Schönberner et al. have rotational velocities of only about 100 km/s. More analyses of these stars are needed to enable a better comparison between theory and observations.

Very recently, objects in the Magellanic Clouds have been observed and their analysis is currently under way (*Kudritzki*, 1985; *Gehren et al.*, 1985). This work tries to obtain new constraints on the theory of stellar evolution of massive stars, which is highly sensitive to mass loss rates (see, for example, *Maeder*, 1981). The mass loss is driven in hot stars by the intense radiation field and is then proportional to the number and opacity of metallic lines, i.e., to the stellar metallicity (*Kudritzki et al.*, 1986, in press), which is supposed to be lower in the LMC and SMC than in our own galaxy (*Dufour*, 1984). Thus, the Magellanic

Clouds offer a new laboratory in which the theories can be tested under conditions different to those pertaining to the Galaxy. However, this is only possible after accurate knowledge of the basic parameters of the stars (T_{eff} , $\log g$, abundances) has been obtained and an observed main sequence has been constructed. This again requires the detailed spectroscopy of a large number of objects.

1.3. – The Subluminous O and B Stars

Subluminous O and B stars may be seen as faint very blue objects in the sky. Subdwarf B stars (sdB) are found in globular clusters and in the field, as can be seen for example in *Newell's* (1977) work. He included a great number of stars, of which only the hottest were sdB. Newell found them to be separated from the Blue Horizontal Branch (BHB) by a gap at $\log T_{\text{eff}} \approx 4.33$ (*Newell gap 2*). *Greenstein and Sargent* (1974) classified the sdB stars as Extended Horizontal Branch (EHB) objects and analyzed a large number of sdO. The $\log g - \log T_{\text{eff}}$ diagram was used in both cases. This allowed the analysis to be carried out without knowledge of the distances. They placed the stars in this diagram and found that the field sdB were Helium poor, and they associated them with Population II stars. However, *Heber* (1986) has shown that most of the field sdB belong to old disk population, although no differences exist between their atmospheric parameters and those of the cluster sdB. The hotter O Subdwarfs are known to belong to the old disk population. Nevertheless, both Newell and Greenstein and Sargent used LTE models which are inadequate for the high temperatures (see *Auer and Mihalas*, 1972).

The first NLTE models appropriate to subluminous O stars were calculated by *Kudritzki* (1976). He separated the domains of LTE and NLTE, showing that most of the sdO should be investigated by means of NLTE models. *Gruschinske and Kudritzki* (1979) showed in addition that sphericity effects can be ignored in these stars. Thus, the models of Kudritzki have been used to analyse the spectra of O and B subdwarfs (e.g. *Kudritzki and Simon*, 1978; *Hunger et al.*, 1981; *Kudritzki et al.*, 1982; *Gruschinske et al.*, 1983; *Heber et al.*, 1984). The picture emerging from this work has been reviewed recently by *Kudritzki* (1985). The Helium abundance of these objects varies from extreme and intermediate Helium rich objects ($Y = N(\text{He})/(N(\text{He}) + N(\text{H})) = 1.0 - 0.5$) to Helium poor ones ($Y < 0.09$). Strikingly Helium poor and intermediate Helium rich objects are clearly

separated in the $\log g - \log T_{\text{eff}}$ diagram by an imaginary line around 40000 K. Thus Helium poor objects are classified as sdB and sdOB types, and the intermediate Helium rich ones as sdO. Moreover, the metal abundances of both groups are different (see, e.g. *Baschek et al.*, 1982; *Kudritzki*, 1985): in intermediate He - rich objects, Silicon is normal, but Nitrogen is enriched and Carbon depleted, strongly pointing to CNO processed material; in Helium poor objects Carbon and Silicon are depleted, and Nitrogen is approximately solar.

The most likely explanation for the abundances in the Helium poor sdB and sdOB is that of gravitational settling (*Vauclair and Vauclair*, 1982). *Groth et al.* (1985) have shown that this mechanism cannot be efficient in the sdO, because these stars develop HeII/HeIII convection zones that penetrate into photospherical layers and prevent diffusion. However, the appearance of these convection zones is dependant on the Helium abundance: once a star has became Helium poor it can no longer develop such a region. This implies that sdO stars cannot evolve from the sdB and sdOB ones, but these groups follow different evolutionary tracks. *Groth et al.* (1985) and *Heber* (1986) have given a scenario for the evolution of the stars after the HB and EHB. The decisive parameter is q , the ratio of the core to the total stellar mass. For $q \leq 0.95$, the star is a HB star, with a double burning shell structure. For $q \geq 0.95$, the star belongs to the EHB and has a single Helium burning shell structure. Following *Groth et al.* and *Heber*, subsequent evolution would proceed as follows:

i) When $q \leq 0.90$, the star ascends the AGB and will evolve into the CPN domain, which we shall discuss in the next section.

ii) When $0.9 \leq q \leq 0.95$, the star will not ascend the AGB, but will turn again bluewards to the domain of the sdO. In its excursion redwards, through regions of low gravity, the diffusion will become ineffective and Helium could appear at the surface due to mass loss or mixing. Finally, they evolve into WD stars with masses $M \leq 0.55M_{\odot}$.

iii) When $q \geq 0.95$, the star behaves like a pure Helium star on the Helium Main Sequence, evolving from the ZAEHB into the sdOB star region, and then into WDs with masses $M \leq 0.50M_{\odot}$.

Unfortunately, this scenario is based on only a few evolutionary calculations from *Gingold* (1976) and *Sweigart et al.* (1974) for the $0.90 \leq q \leq 0.95$ tracks and from *Castellani* (1985, cited in *Groth et al.*, (1985), $q = 0.99$) and *Paczynski* (1971, $q = 1.0$). Moreover, these calculations do not include mass loss or mixing, effects that could be of first order in the explanation of the observed abundance patterns.

Spectroscopically the situation is slightly better as the number of carefully analyzed objects (most of them only for T_{eff} , $\log g$ and Helium abundance) is greater than 30. In addition, *Schönberner and Drilling* (1984) have derived temperatures and gravities for 12 very hot subdwarfs from low resolution IUE spectra. Their objects lie in the zone that the most evolved subdwarfs should occupy on their way to the WD stage. *Husfeld* (1986) analyzed in detail three of the four objects classified by *Schönberner and Drilling* as Helium rich (they could only distinguish between Helium "normal" and "rich" objects due to the nature of their analysis). Although the values given by *Husfeld* for $\log g$ and T_{eff} are somewhat different to those of *Schönberner and Drilling*, they lie in the same region of the diagram. *Husfeld* concludes that his objects - in fact they are all extremely Helium rich - have probably evolved from the AGB with masses only slightly smaller than those of CPN (q slightly greater).

Although the above described scenario seems to be coherent and in general agreement with the observations, it is highly speculative and constitutes more a first picture of the situation (for example, details such as *Newell's gap 2*, the explanation of which remains unclear (*Heber et al.*, 1986), are not considered). Therefore much work has still to be done. Not only are there too few theoretical evolutionary calculations but detailed spectroscopy should also test the prediction of *Groth et al.* (1985) that Helium poor objects exist in the domain of the Helium rich ones; abundances of Helium and heavy elements are needed to put constraints on the different physical mechanisms that can act in each phase (diffusion, mass loss, Helium shell flashes, etc.); finally the accurate placement of stars in the $\log g$ - $\log T_{\text{eff}}$ diagram must be continued.

I.4. – The Central Stars of Planetary Nebulae

The Central stars of Planetary Nebulae (CPN) are very blue objects of various spectral types. They are the progenitors of the planetary nebulae in whose centres they can be usually seen.

These stars are often faint objects whose spectra, because of contamination by nebular radiation, are difficult to obtain and analyze. Moreover, only a fraction of the stars, with sdO spectral type, have absorption spectra that can be analyzed with present techniques. For all these reasons, only a very few CPN have been analyzed with quantitative spectroscopical techniques (*Mendez et al.*, 1985).

As a consequence the Zanstra and Stoy methods have been widely used in the past (see *Pottasch*, 1984). These methods however, give only an estimate of the stellar temperature and are inadequate for detailed analysis. As an example, the Zanstra discrepancy may be cited: The temperature obtained when this method is applied to Hydrogen may be very different to that obtained when it is applied to HeII. The discrepancy is probably due to differences in the optical thickness of the PN for H and HeII (*Kaler*, 1983).

Another method is the use of the spectral distribution or of colour temperatures from IUE data (see *Kaler and Feibelman*, 1985). They are very difficult to apply to hot stars (such as CPN), as the theoretical energy distributions are insensitive to the effective temperature at wavelengths greater than the flux maximum. This insensitivity may be seen in the cited work of Kaler and Feibelman. Unfortunately, quantitative spectroscopy is difficult for the reasons given above. Moreover, the lack of HeI lines in most of the CPN, due to the high temperatures or to nebular emission, makes it difficult to determine the effective temperature with this method. The temperature must then be deduced from the fit of the Balmer line profiles and is sometimes in contradiction with the one derived from the lack of HeI lines (*Mendez et al.*, 1985): as for some O stars, the calculated Balmer line profiles are too shallow.

For all these reasons, these stars have not yet been accurately positioned in the HR diagram or in the $\log g - \log T_{\text{eff}}$ one, which, as seen in the preceding sections, is an important pre-condition for the study of their evolutionary status and properties.

As indicated in the last section, stars on the Horizontal Branch with a ratio q of core mass to total stellar mass less than 0.9 continue their evolution by ascending the Asymptotic Giant Branch (AGB). The star expands and cools and becomes a red giant of very high luminosity (see, e.g., the review of *Iben and Renzini*, 1983). The nebula is probably formed from the material ejected during this phase and/or at its end, although the mechanism is still unknown (see *Iben*, 1984). However, theoretical models of stars in the AGB suffer numerous Helium shell flashes (*Schönberner*, 1979) and cross a region of instability in the HR diagram, with strong winds (see *Pottasch*, 1984, chapter IX). These facts are probably related to the PN ejection. When leaving the AGB, the star evolves towards higher temperatures with a constant luminosity that depends only on the core mass ("core-mass luminosity" relation). Finally, the star is hot enough to ionize the nebula which becomes visible.

Models of CPN have been calculated by *Paczynski* (1971) and *Schönberner* (1979). These stars have an inactive core of carbon-oxygen surrounded by a Helium shell, and a Hydrogen shell that provides most of the luminosity, and finally by a low mass envelope. The star then evolves rapidly through the constant luminosity phase, becoming hotter as it contracts (the envelope shrinks as the burning shell advances). When the fuel is substantially exhausted the star decreases in luminosity and cools evolving towards the white dwarf stage. The theoretical tracks of *Paczynski* and *Schönberner* agree qualitatively, although the evolutionary times of *Paczynski* are too short. The nebula expands and becomes less luminous, until at the end no nebula can be seen.

One important point is that a Helium shell flash may occur during the CPN evolution (*Iben et al.*, 1983; *Schönberner*, 1983), expanding the envelope and lowering the stellar temperature. The star returns to the giant phase and evolves once more as before at constant - but slightly higher - luminosity. A total of 10% (*Iben et al.*, 1983) or 20% (*Schönberner*, 1983) of the CPN should suffer this so called "last Helium shell flash".

Comparison of these theoretical tracks and their predictions with observations is not an easy task since the position of the stars in the $\log L - \log T_{\text{eff}}$ is not very accurate due to uncertainties in the determination of temperatures (the Zanstra method is usually used) and luminosities (distances are required). Moreover, the study of the abundances is problematic, not only because of the

difficulty in studying the stellar spectra, but also because no clear predictions are derived from the theory, as a small Hydrogen rich envelope always remains in the calculations (*Schönberner, 1979; Iben et al., 1983*).

Renzini (1979) compared observed CPN with tracks of Paczynski and found that the CPN should have masses between 0.55 and (at least) $1.2M_{\odot}$, the less luminous CPN being more massive than the brighter ones. Thus these less luminous CPN should have higher abundances of He and N compared with the others, as they had more massive progenitors. The prediction is then extended to their PN because their abundances can be studied more easily.

The conclusions of *Schönberner (1981)* are different. He found a surprisingly narrow CPN mass distribution (narrower than that of white dwarfs). From his discussion it follows that most of the CPN ($\approx 80\%$) have masses between 0.55 and $0.64M_{\odot}$, and no correlation is to be found between the brightness and the abundances of the PN.

Kaler (1983) finds again a wider distribution of masses, from 0.55 (a lower limit) to $1.0M_{\odot}$. Although most of the differences between his and Schönberner's results can be explained by the different assumptions of both authors, a small discrepancy remains. Kaler's study of abundance ratios leads him to the conclusion that the N/O ratio increases with decreasing stellar brightness and probably correlates with the He/H ratio, again in contradiction with Schönberner.

In his work Kaler gives error bars in his figures, which allows the inaccuracies present in the study of these parameters (temperatures, abundances, luminosities) to be appreciated. However, only one CPN has been analyzed for metallic abundances by means of quantitative spectroscopy (*Husfeld, 1986*) and only 12 more have been investigated for temperatures, gravities and Helium abundances (*Mendez et al., 1985*). These last authors found that their two CPN with higher gravities (probably the most evolved) are Helium poor, an indication of depletion, and that these CPN lie on a mass range between 0.55 (or perhaps slightly less) and $0.60M_{\odot}$, thus reinforcing the criterium from Schönberner. However, more data are needed before firm conclusions can be drawn that resolve the controversies outlined above. In particular, the accurate placement of a representative number of CPN in the HR diagram is urgently required.

1.5. – Objectives of the Present Work

In the preceding sections we have described those groups of very hot stars that can be analyzed with current spectroscopical techniques, thus allowing an accurate placement of the objects in the $\log g - \log T_{\text{eff}}$ plane and then in the usual HR diagram. This constitutes the first requirement for the theoretical interpretation of their evolutionary history. In addition, quantitative spectroscopy gives detailed information about the photospheric structures and about relevant atomic processes. This information may be then used in other related areas, such as stellar interiors (evolution, convection) and upper layers of the atmospheres (mass loss, stellar winds) and to distinguish effects that may be important in the photospheres (sphericity, velocity fields).

However, these studies are very expensive as they require very sophisticated computations. Thus the search for new techniques that reduce the computational effort, while maintaining (or even increasing) the accuracy, is a necessity in this field.

Recently, a new technique (described in the next chapter) has been developed. It has been called the Accelerated Lambda Iteration (*Werner and Husfeld, 1985*) and fulfils the above requirements. It has been tested by the aforementioned authors by comparing it with previous results.

The promising results from Werner and Husfeld encouraged us to extend the tests and calculations to problems for which present techniques were not powerful enough.

From the theoretical point of view, some problems were suitable for this purpose. The model atom of Hydrogen had been treated only with five NLTE levels not all of them being radiatively coupled. The lines were considered to have a depth-independent profile, the only broadening mechanism considered being that of thermal Doppler broadening. However, it is known that Stark broadening is important in early type stars due to the high densities. The effect of these approximations had been at best only estimated, so that it was decided to apply the new technique to these problems.

Similar comments may be made for ionized Helium, so it was also decided to perform the same calculations for this ion as for Hydrogen and to then solve the full overlap problem between the lines of both elements, a problem that had never before been treated. And, of course, it is always possible to gain new experience when applying new techniques to unsolved problems.

From the observational point of view, two effects could be related to these calculations. First, the discrepancy between observed and calculated line cores of the Balmer lines in slow rotators (the effect in other stars probably being masked by rotation), which becomes especially important in CPN, as we have seen. Second, the $\lambda 4686$ emission of HeII in some stars could be at least partially, explained by the overlap of H and HeII through the Bowen mechanism.

Finally, one more reason are the new observational techniques that allow profiles to be measured with much greater accuracy than before. Our work should give information concerning the required detail necessary in such calculations, in order that the accuracy of the new observational material be matched.

CHAPTER II

Line Formation in Stellar Photospheres

In this chapter we wish to present schematically the techniques used to solve line formation problems (i.e., the simultaneous solution of the equations determining the occupation numbers and the radiation field). Special emphasis is given to techniques appropriated to the stars described in the preceding chapter.

The atmosphere of a star may be defined as the layer from which the energy produced in the stellar core leaves the star and reaches outer space. It is implicit in this definition that no energy is produced in the atmosphere: the dominant physical process is the transfer of energy. We will assume that there is no convective motion, so that this energy is transported only radiatively. This hypothesis is known as RADIATIVE EQUILIBRIUM. Moreover, we will suppose PLANE-PARALLEL GEOMETRY and HYDROSTATIC EQUILIBRIUM. With these hypotheses we are actually limited to the photosphere, the region where most of the optical spectrum comes from.

Sections II.1. and II.2. are devoted to the transfer equation and its solution. Sections II.3. and II.4. are dedicated to the statistical equilibrium equations. In sections II.5. to II.8., the classical methods for the solution of these coupled equations are presented. A more extensive discussion of all these topics can be found in *Mihalas (1978)*. Sections II.9. and II.10. treat the more recently developed perturbation methods, Scharmer's method and the Accelerated Lambda Iteration.

II.1. – The Equation of Transfer

With the above assumptions we can derive the equation governing the passage of radiation through the photosphere. We start by defining the specific intensity I_ν

$$\delta \epsilon = I_\nu \, dS \cos\theta \, d\omega \, d\nu \, dt \quad (2.1)$$

i.e., I_ν is the amount of energy per unit bandwidth, $d\nu$, travelling in a specific direction through unit area, $dS \cos\theta$, into unit solid angle, $d\omega$, within unit time dt . Its units are then $\text{ergs cm}^{-2} \text{ s}^{-1} \text{ Hz}^{-1} \text{ sr}^{-1}$.

When radiation travels through a layer of material of thickness z in direction μ ($= \cos\theta$), the change of the intensity is equal to the difference between the energy emitted and absorbed by the material:

$$\mu (dI_\nu/dz) = \eta_\nu - \chi_\nu I_\nu \quad (2.2)$$

where the energy released is given by the emissivity η_ν (which has units of $\text{erg cm}^{-3} \text{ s}^{-1} \text{ Hz}^{-1} \text{ sr}^{-1}$) and the absorbed energy is given by the product $\chi_\nu I_\nu$. The absorption coefficient χ_ν has units of cm^{-1} .

By defining the optical thickness

$$d\tau_\nu = - \chi_\nu dz \quad (2.3)$$

and the source function

$$S_\nu = \eta_\nu / \chi_\nu \quad (2.4)$$

we may write the transfer equation in the standard form

$$\mu (dI_\nu/d\tau_\nu) = I_\nu - S_\nu \quad (2.5)$$

II.2. – Formal Solution of the Transfer Equation

If S_ν is a given quantity, or depends on the radiation field only through the scattering integral (the integral of the intensity over frequency and angle that represents the scattering processes, see *Mihalas*, 1978, pg.152), equation (2.5) may be solved directly. Among the many techniques available, the ones developed by *Feautrier* (1964), together with the Eddington variable factors from *Auer and Mihalas* (1970) and the variation due to *Rybicki* (1971a), are the most powerful.

II.2.1. – Feautrier's Scheme

In this method the transfer equation is written separately for outgoing ($0 \leq \mu \leq 1$) and incoming ($-1 \leq \mu \leq 0$) radiation

$$\pm \mu (dI_v/d\tau_v) = I_v(\tau_v, \pm \mu) - S_v = I_v^\pm - S_v \quad (2.6)$$

where we have assumed that S_v is symmetric in μ , i.e., I_v and χ_v have the same μ -dependence (usually they are supposed to be isotropic). We define now the symmetric and antisymmetric averages

$$u_v = \frac{1}{2} (I_v^+ + I_v^-) \quad (2.7)$$

$$v_v = \frac{1}{2} (I_v^+ - I_v^-) \quad (2.8)$$

Adding and subtracting the two equations represented by (2.6)

$$\mu (dv_v/d\tau_v) = u_v - S_v \quad (2.9)$$

$$\mu (du_v/d\tau_v) = v_v \quad (2.10)$$

Substituting (2.10) into (2.9) we obtain

$$\mu^2 (d^2 u_v / d\tau_v^2) = u_v - S_v \quad (2.11)$$

Equation (2.11) requires two boundary conditions to allow its solution. We will suppose that at the outer boundary neither material nor incoming radiation from space are present, so that the condition is that at $\tau_v = 0$

$$\mu (du_v/d\tau_v) = u_v(0) \quad (2.12)$$

At the inner boundary, $\tau_{\max}$, we will assume the diffusion approximation, valid for great τ_v

$$\mu [du_v/d\tau_v]_{\tau_{\max}} = \mu (1/\chi_v |dB_v/dz|)_{\tau_{\max}} \quad (2.13)$$

All variables are now discretized and equation (2.11) is replaced, for each fixed value of μ and ν , by a difference equation at each point in the atmosphere. The scattering integral in the source function is replaced by a quadrature sum. These quadrature sums contain all frequencies and angles, and not only those for which the difference equation was developed, thus coupling all frequency - angle points at each depth.

We group now all frequency - angle components and obtain at each depth d a matrix equation

$$- \mathbf{A}_d \mathbf{u}_{d-1} + \mathbf{B}_d \mathbf{u}_d - \mathbf{C}_d \mathbf{u}_{d+1} = \mathbf{L}_d \quad (2.14)$$

where variables in boldface are matrices (italics) or vectors.

The system, including the boundary conditions (2.12) and (2.13), has a block tridiagonal structure and is solved in a forward - backward substitution using standard techniques. The solution time in Feautrier scheme scales as cDM^3N^3 , where D is the number of depth points and M and N are the number of angle and frequency points respectively.

II.2.2. - Variable Eddington Factors

Auer and Mihalas (1970) pointed out that in most stellar atmospheres problems only the mean intensity J_ν is needed. By integrating equation (2.11) over angle we obtain

$$d^2(f_\nu J_\nu)/d\tau_\nu^2 = J_\nu - S_\nu \quad (2.15)$$

where f_ν is the so called *variable Eddington factor*, defined to be

$$f_\nu = K_\nu / J_\nu \quad (2.16)$$

and K_ν is the second moment of the radiation field

$$K_\nu = \frac{1}{2} \int_{-1}^{+1} I_\nu \mu^2 d\mu \quad (2.17)$$

The corresponding boundary conditions for equation (2.15) are now

$$\left[d^2(f_\nu J_\nu) / d\tau_\nu^2 \right]_{\tau_\nu=0} = h_\nu J_\nu(0) \quad (2.18)$$

with

$$h_\nu = H_\nu(0) / J_\nu(0) \quad (2.19)$$

at the outer boundary, and at the inner one

$$\left[d(f_\nu J_\nu) / d\tau_\nu \right]_{\tau_{\max}} = \frac{1}{2} \left[1/\chi_\nu \left| dB_\nu / d\tau_\nu \right| \right]_{\tau_{\max}} \quad (2.20)$$

For a given f_ν solution of equation (2.18) together with conditions (2.19) and (2.20) scales only as cDN^3 . However, f_ν must be estimated and the whole process iterated, so that the total time after L iterations is $L(cDN^3 + c'DMN)$. If L remains small, this time scales favourably compared with the time taken by the Feautrier method.

II.2.3. - Rybicki's Scheme

The solution time for the two methods above increases very rapidly with the number of frequency points. Rybicki realized that in the case of COMPLETE REDISTRIBUTION (photons are scattered with frequency ν' independent of the incident frequency ν) the source function would depend only on J , where

$$J = \int \phi_\nu J_\nu d\nu \quad (2.21)$$

ϕ_ν being the line profile function.

Now the depths are grouped and we have a matrix equation for each angle - frequency point i of the form

$$T_i u_i + U_i J = K_i \quad (2.22)$$

The system is completed with the equations defining J (one equation at each depth point) .The time to solve the system scales as $cD^2MN + c'D^3$, only linearly with MN .

II.3. – The Statistical Equilibrium Equations

To solve the transfer equation we have assumed that the source function was a given quantity (except for the scattering integral). This is equivalent to the statement that we know the detailed populations of the atomic levels, because only thus are we able to calculate the emission and absorption coefficients.

Consider a volume element in the atmosphere. The change in the number density of a given state i of a chemical species k will be equal to the net flux of such particles flowing through the volume element with velocity $\mathbf{v}$ plus the net rate at which the population of the state changes by atomic processes

$$\partial n_{ik} / \partial t = -\nabla(n_{ik}\mathbf{v}) + \sum_{j \neq i} (n_{jk} P_{ji} - n_{ik} P_{ij}) \quad (2.23)$$

where P_{ij} is the net rate from level i to j .

If we assume that our atmospheres are STATIC and in STEADY STATE equation (2.23) reduces to

$$n_{ik} \sum_{j \neq i} P_{ij} - \sum_{j \neq i} n_{jk} P_{ji} = 0 \quad (2.24)$$

We close the system represented by equation (2.24) by demanding, e.g., that the total number of particles of species k equals its desired fractional abundance

$$\sum_i n_{ik} = \epsilon_k (n_{\text{tot}} - n_e) \quad (2.25)$$

where n_{tot} is the total particle number density and n_e is the electron number density. The system may be written finally in the form

$$\mathbf{A} \mathbf{n} = \mathbf{b} \quad (2.26)$$

Here vector $\mathbf{b}$ contains only zeroes and the right term of equation (2.25); vector $\mathbf{n}$

contains the unknown population numbers. The elements of matrix **A** are the rates P_{ij} , the final row describing e.g. number conservation (2.25).

II.4. – Radiative and Collisional Rates

To calculate the rates P_{ij} we must consider the microscopic processes that determine the population of a state: excitation and ionization by encounters with other particles and by absorption of photons and the corresponding inverse processes.

In stellar atmospheres it is supposed that all particles have a MAXWELLIAN DISTRIBUTION of velocities with a COMMON TEMPERATURE. As a consequence electrons are faster than any other particles and usually only electron collisions are considered (not a necessary assumption). With this hypothesis the collisional rate from level i to level j may be written (*Mihalas*, 1978, pp.131 – 133)

$$C_{ij} = C_0 T^{1/2} n_e e^{-(E_0/kT)} \Gamma_{ij}(T) \quad (2.27)$$

where n_e and T are the electron density and temperature, E_0 is the threshold energy of the transition and k is the Boltzmann constant. The constant C_0 is

$$C_0 = \pi a_0^2 (8k/m\pi)^{1/2} = 5.465 \times 10^{-11} \text{ cm}^2 (\text{erg K}^{-1} \text{ gr}^{-1})^{1/2} \quad (2.28)$$

a_0 being the Bohr radius and m the electron mass. The numerical values are taken from *Allen* (1973).

$\Gamma_{ij}(T)$ is an integral function containing the cross section in the integrand, and constitutes the main problem in determining C_{ij} , because of resonances in the collisional processes (mainly autoionization).

An alternative expression for equation (2.27) is (*Mendoza*, 1983)

$$C_{ji} = 8.631 \times 10^{-8} n_e / (T^{1/2} g_j) \int_0^{\infty} \Omega_{ij} e^{-E/kT} d(E/kT) \quad (2.29)$$

It must be noted that now we have written C_{ji} instead of C_{ij} as in equation (2.27). The advantage of equation (2.30) is that Ω_{ij} can usually be well approximated by a

constant value Ω_m (and $\Omega_m = 1$ is normally a good choice), so that an estimate for excitation rates is always available.

Where neither experimental data nor theoretical calculations exist, some approximate expressions may be used, e.g., *van Regemorter's* (1962) formulae for excitation (only if the oscillator strength f_{ij} is different from zero), and those given by *Seaton* (1962), *Lotz* (1968) and *Burgess and Chidichimo* (1983) for ionization.

The probabilities of absorption and emission of photons between two bound levels, i and j , are related to the Einstein coefficients for absorption and spontaneous and stimulated emission, B_{ij} , A_{ji} , B_{ji} . The first of these is defined so that the rate at which the energy is removed from a beam of intensity I_ν is

$$n_i B_{ij} h\nu_{ij} (d\omega/4\pi) \phi_\nu I_\nu = \chi'_\nu I_\nu \quad (2.31)$$

ϕ_ν being the absorption line profile and χ'_ν is the absorption coefficient per unit solid angle $d\omega$. The coefficient of spontaneous emission is defined so that the energy emitted by this process is

$$\eta_\nu^{sp} = n_j A_{ji} h\nu_{ij} (d\omega/4\pi) \psi_\nu \quad (2.32)$$

where ψ_ν is the emission line profile; the rate at which energy is emitted through stimulated emission processes is

$$\eta_\nu^{st} = n_j B_{ji} h\nu_{ij} (d\omega/4\pi) \psi_\nu I_\nu \quad (2.33)$$

Under the usual assumption of COMPLETE REDISTRIBUTION the emission and absorption profiles are equal and the Einstein coefficients are related through the Einstein relations

$$g_i B_{ij} = g_j B_{ji} \quad (2.34)$$

$$A_{ji} = 2h\nu^3/c^2 B_{ji} \quad (2.35)$$

where g_i , g_j are the statistical weights of levels i and j .

The rates at which levels i and j are populated and depopulated may be deduced from equations (2.31) to (2.35). Thus we obtain for the upward rates

$$n_i R_{ij} = n_i 4\pi \int \sigma_{ij} (J_\nu/h\nu) d\nu \quad (2.36)$$

with

$$\sigma_{ij} = B_{ij} (h\nu_{ij}/4\pi) \quad (2.37)$$

and, for the downward rates

$$n_j R_{ji} = n_j (n_i/n_j)^* [4\pi \int (\sigma_{ij}/h\nu) (2h\nu^3/c^2 + J_\nu) e^{-h\nu/kT} d\nu] \quad (2.38)$$

in both cases after integration over the angular variables.

For the bound - free transitions similar expressions may be derived.

The coupling between the radiation field and the occupation numbers can now be clearly seen: the occupation numbers are determined by equation (2.24), which assumes knowledge of the radiation field in equations (2.36) and (2.38). However, to know the radiation field we must solve the equation of radiative transfer, that is, we must know the thermal part of the source function that depends on the occupation numbers through equations (2.31) to (2.33). The techniques to solve this coupled problem, which constitutes the main difficulty in radiative transfer problems in stellar atmospheres, will be described in the next sections.

II.5. - Local Thermodynamic Equilibrium (LTE)

The most simple solution to the coupling between radiation field and occupation numbers is to introduce some new constraints to determine independently one group of variables. Under the hypothesis of LTE the occupation numbers are not given by equation (2.24), but by the equations of thermodynamic equilibrium at the local electron temperature. The relative populations between any two levels i, j of some ion are given by the Boltzmann equation

$$(n_i/n_j)^* = (g_i/g_j) e^{-(\chi_i - \chi_j)/kT} \quad (2.39)$$

where χ_i and χ_j are the excitation energies with respect to the ground level. The relative populations between any two successive stages of ionization of some chemical species are given by the Saha equation, usually written as the population of level i of stage $(k-1)$ relative to population of ground level of stage k

$$(n_{i,(k-1)} / n_{0,k}) = n_e (g_{i,(k-1)} / g_{0,k}) C_I T^{-3/2} e^{(\chi_{I,(k-1)} - \chi_{i,k-1})/kT} \quad (2.40)$$

where the constant C_I is

$$C_I = 1/2 (h^2 / 2\pi m k)^{3/2} = 2.070 \times 10^{-16} \text{ (erg s}^2 \text{ gr}^{-1} \text{ K)}^{1/2} \quad (2.41)$$

and $\chi_{I,(k-1)}$ the ionization energy of the ionization stage $(k-1)$. Numerical values are taken again from *Allen* (1973).

The system may be closed again by equation (2.25), and the absolute occupation numbers can then be determined. Moreover, in LTE the source function is given by the Planck function. The only unknown variable, the radiation field, can now be calculated by mean of the methods described in II.2.

II.6. – The Lambda Iteration

Another simple method might be to solve the problem iteratively. We start with some estimate of the source function and solve for the radiation field in the radiative transfer equation. Since the radiation field is now known we can calculate the occupation numbers by means of the statistical equilibrium equations. The whole process is iterated until convergence is reached.

The method is named after the lambda operator, the representation of the integral solution of the transfer equation, which is repeatedly applied.

$$J_\nu(\tau_\nu) = \Lambda_{\tau_\nu}[S_\nu] \quad (2.42)$$

However, the lambda iteration does not converge. The corrections may be small, but they remain constant iteration after iteration, and the solution stabilizes.

The problem may be described physically as follows: with the lambda iteration information propagates approximately only over optical depth unity after each iteration. Thus, if some frequency is optically thin photons escape from layers in which the occupation numbers are determined by collisional processes and the lambda iteration converges. However, if it is optically thick, photons must be followed through to the optical depths in which they drive the populations. For some transitions the number of iterations becomes prohibitive.

II.7. – The Equivalent Two Level Atom

Suppose that we have a model atom with only two levels connected by a line. Then it is possible to eliminate analytically the ratio of the levels appearing in the source function by using the statistical equilibrium equations: this is the so called *two level atom*.

But such a model atom is of course unrealistic. Other bound – free and bound – bound transitions will in general be present and, although possible, it is useless to eliminate all population ratios from the corresponding source functions: the expressions would become too complicated to be useful.

The chosen approximation is to suppose that the source function in the line is principally determined by processes between the two levels and between these levels and the continuum. The influence of all other transitions is grouped together in net brackets giving the effect of the upward and downward rates for each transition and held fixed at its value from the previous iteration. Thus it is possible to obtain analytical formulae for each line source function, that are formally identical to those derived for the two level atom (For this reason the method is called *the equivalent two level atom approach*).

An iteration procedure is nevertheless still needed: we start with some estimation of the atomic populations and, regarding the source function as known, solve for the radiation field in each considered transition. With this first estimate we can compute radiative rates and, by assuming initially that the net brackets are zero,

one radiative transfer equation may be solved for each transition using standard methods. Now the statistical equilibrium equations are solved and better estimates of the population numbers, the rates and the net brackets are obtained. The whole process is again iterated until convergence is reached.

The main difficulty in this approach is the implicit assumption that the interdependence between different radiative transitions is weak. This can lead to instabilities or inconsistencies in the solution and limits the applicability of the method to resonance lines involving metastable levels and to the layers in which the terms coupling both levels with themselves and/or with the continuum dominate over all other terms.

II.8. – The Complete Linearization Method

The methods we have seen until now are not powerful enough to treat the whole multilevel problem. In the linearization method (*Auer and Mihalas, 1969*) the dependence of the population numbers at each point in the atmosphere on the radiation field at each frequency and depth, and vice versa, is treated explicitly by considering a linear expansion of the equations about the current solution. Thus, suppose that the vector ξ describes the true run of all variables with depth. The vector ξ is still unknown but

$$f(\xi) = 0 \quad (2.43)$$

where $f(\xi)$ represents the whole system of transfer plus statistical equilibrium equations. Now, if ξ^0 is some current estimate of ξ , we suppose that

$$\xi = \xi^0 + \delta\xi \quad (2.44)$$

which of course means that

$$f(\xi^0 + \delta\xi) = 0 \quad (2.45)$$

Finally, by expanding $f(\xi)$ about ξ^0 we obtain

$$f(\xi^0 + \delta\xi) = f(\xi^0) + (\partial f/\partial \xi) \delta\xi = 0 \quad (2.46)$$

The transfer equation was written (equations 2.4, 2.15)

$$(\partial^2(f_{\nu}J_{\nu})/\partial \tau_{\nu}^2) = J_{\nu} - (\eta_{\nu}/\chi_{\nu}) = L \quad (2.47)$$

By linearizing equation (2.47)

$$(\partial^2(f_{\nu}J_{\nu})/\partial \tau_{\nu}^2) - \delta J_{\nu} + (\delta\eta_{\nu}/\chi_{\nu}^0) - \delta\chi_{\nu}\{\eta_{\nu}^0/(\chi_{\nu}^0)^2\} = L^0 \quad (2.48)$$

where χ_{ν}^0 , η_{ν}^0 and L^0 are current estimates and the $\delta\eta_{\nu}$, $\delta\chi_{\nu}$ are proportional to the δn_i - equations (2.31), (2.32), (2.33) . Moreover, these may be written

$$\delta n_d = \sum_{k=1,K} [\partial n_d/\partial J]_k \delta J_k \quad (2.49)$$

and it is possible to find an analytical expression for the $(\partial n_i/\partial J)$. By eliminating the $\delta\eta_{\nu}$, $\delta\chi_{\nu}$ in equation (2.48) in terms of the δJ_{ν} , we obtain finally at each depth d an equation for δJ in the standard Feautrier form

$$-A_d \delta J_{d-1} + B_d \delta J_d - C_d \delta J_{d+1} = L_d \quad (2.50)$$

Here δJ_d is a vector describing the frequency run of the corrections to the mean intensity at depth d. The boundary conditions are treated in a similar way before being included in the system.

The problem can be now initialized starting, for example, with LTE populations, and a first estimate of the radiation field is calculated. This is now used to calculate photoionization rates and the statistical equilibrium equations are solved, keeping the lines in detailed balancing. The lines are then treated with the equivalent two level atom approach and thus new occupation numbers are obtained. After some few iterations the current estimates of the radiation field and atomic populations are adopted as initial values for the linearization method. Equation (2.50) is solved for the transitions of interest and the rates are kept fixed for all other transitions at their equivalent two level atom values. The δJ 's from equation (2.50) are used to obtain better estimates of the radiation field and the statistical equilibrium equations are solved once more. The procedure is iterated until some convergence criterium is satisfied.

A convergence of 10^{-4} in the occupation numbers is usually achieved after only a small number of iterations, but equation (2.50) must be solved using Feautrier's method and, because matrices A , B and C are full, it becomes very expensive for increasing number of frequencies. In addition, since these matrices are of dimension ($n_{\text{freq}} \times n_{\text{freq}}$) the description of the radiation field is necessarily limited.

For these reasons *Auer and Heasley* (1976) developed a method based on the Rybicki scheme. The linearized transfer equation (2.46) may be written

$$T_k \delta J_k + L_k \delta n_l + U_k \delta n_u = R_k \quad (2.51)$$

Here it is assumed that at frequency k only the transition t between levels l and u contributes to the emission and absorption processes.

Now we define the variation in the rates of transition t at depth d as

$$(\delta Z_t)_d = n_{l,d} \delta R_{lu,d} - n_{u,d} \delta R_{ul,d} \quad (2.52)$$

δZ_t is of course a function of δJ_k within the transition, so that substituting in (2.51)

$$\delta Z_t + A_t \delta n_l + B_t \delta n_u = C_t \quad (2.53)$$

and, because the δn are also a function of the δJ_k 's, one may write

$$\delta n_m = \sum_t D_{mt} \delta Z_t \quad (2.54)$$

Substituting in (2.53) we obtain finally the system

$$\begin{aligned} E_t \delta Z_t &\equiv (I + A_t D_{lt} + B_t D_{ut}) \delta Z_t \\ &= C_t - A_t \sum_{t' \neq t} D_{lt'} \delta Z_{t'} - B_t \sum_{t' \neq t} D_{ut'} \delta Z_{t'} \end{aligned} \quad (2.55)$$

We have one equation like (2.55) for each transition at each depth point in the atmosphere, and the system is too large to solve for δZ_t directly.

We start by obtaining an initial estimate for the δZ_t by solving the equation $E_t \delta Z_t^0 = C_t$. Keeping E_t fixed, we substitute the current estimates of δZ_t on the right hand side of (2.55), and obtain better ones. The process is iterated, but only until a coarse accuracy has been achieved because we then use the δZ_t 's simply to update the radiative rates. The statistical equilibrium equations are solved once again and new occupation numbers are calculated. The overall convergence is determined by this last iteration cycle, and the computing time increases only linearly with the number of frequency points.

This method has proved to be very efficient and stable and can deal with very complicated multilevel cases on line formation problems, as here the limit is imposed by the number of transitions.

II.9. - Perturbation Methods

Another completely different approach to solve the problem is provided by the perturbation method originally developed by Cannon (1973a,b) to obtain accurate solutions to the transfer equation (which is equivalent to the line formation problem in the two level atom formulation).

The transfer equation may be rewritten

$$S_v(\tau_v) = \Lambda_{T_v}(S_v) + q(\tau_v) \quad (2.56)$$

The Λ operator in equation (2.56) is not the same as in equation (2.42), but in both cases it is an integral operator involving angle and frequency integration. The integrals are usually replaced by quadrature sums. Cannon's idea was to write equation (2.56) in the form

$$S_v(\tau_v) = \Lambda_{T_v}^*(S_v) + (\Lambda_{T_v} - \Lambda_{T_v}^*)(S_v) + q(\tau_v) \quad (2.57)$$

where the new operator $\Lambda_{T_v}^*$ is calculated only with a reduced number of quadrature points and equation (2.57) may now be solved iteratively or through a perturbation series. The computing time is determined by the approximate operator $\Lambda_{T_v}^*$, but the accuracy is that of the more expensive one, Λ_{T_v} .

Scharmer (1981) applied the idea of an approximate operator to equation (2.42). He writes

$$J_{\nu}(\tau_{\nu}) = \Lambda_{\tau_{\nu}}^*(S_{\nu}) + (\Lambda_{\tau_{\nu}} - \Lambda_{\tau_{\nu}}^*)(S_{\nu}) \quad (2.58)$$

Scharmer's idea is to look for new and simpler forms of the $\Lambda_{\tau_{\nu}}^*$ operator. He uses two already well known approximations. The first one, called the *core saturation method* (Rybicki, 1971b), assumes that for some frequency ν each emitted photon is immediately absorbed at the same point, so that (after integrating over angle)

$$J_{\nu}(\tau_{\nu}) = S_{\nu}(\tau_{\nu}) \quad (2.59)$$

This approximation is applied only for frequencies such that

$$\tau_{\nu} \geq \gamma \quad (2.60)$$

where γ has a value of order unity. The second one is the Eddington - Barbier relation, from which we obtain

$$J_{\nu}(\tau_{\nu} < \gamma') = 1/2 S_{\nu}(\tau_{\nu} = \gamma') \quad (2.61)$$

Setting $\gamma = \gamma'$, we can write for the approximate operator

$$\Lambda_{\tau_{\nu}}^* = \begin{cases} 1 & \tau_{\nu} \geq \gamma \quad (\text{core approximation}) \\ 1/2 S_{\nu}(\tau_{\nu} = \gamma) & \tau_{\nu} < \gamma \quad (\text{wing approximation}) \end{cases} \quad (2.62)$$

The radiation field can now be estimated and its value substituted in the statistical equilibrium equations. It is important that the radiation field at τ_{ν} depends only on local values or on values at $\tau_{\nu}' > \tau_{\nu}$, so that the matrix in equation (2.26) is block diagonal and the vector $\mathbf{n}$ may be found at each depth with a minimum of effort.

Scharmer (1981) applied the operator in (2.62) to a two level atom. In the application to the multilevel case (Scharmer and Carlsson, 1985) a more complicated operator is used, allowing for non local coupling with depth points $\tau'_v < \tau_v$ but losing the greatest advantage of the operator $\Lambda_{\tau_v}^*$.

II.10. – The Accelerated Lambda Iteration

Werner and Husfeld (1985) used the operator (2.62) to develop a new method called the *Accelerated Lambda Iteration* (ALI), because the wing approximation resembles the lambda iteration and the core approximation accelerates the convergence in those regions where the lambda iteration fails.

We start as usual with some estimate of the occupation numbers. We then introduce equations (2.58) and (2.62) in the statistical equilibrium equations so that the radiative rates may now be written (see 2.36, 2.38)

$$\begin{aligned} R_{ij} &= 4\pi \int_0^{\infty} (\sigma_{ij}/h\nu) J_\nu d\nu \\ &= 4\pi \int_0^{\infty} (\sigma_{ij}/h\nu) \{ \Lambda_{\tau_v}^*(S_\nu) + (\Lambda_{\tau_v} - \Lambda_{\tau_v}^*)(S_\nu) \} d\nu \end{aligned} \quad (2.63)$$

$$\begin{aligned} R_{ji} &= 4\pi (n_i/n_j) \int_0^{\infty} (\sigma_{ij}/h\nu) (J_\nu + 2h\nu^3/c^2) e^{-h\nu/kT} d\nu \\ &= 4\pi (n_i/n_j) \int_0^{\infty} (\sigma_{ij}/h\nu) \{ \Lambda_{\tau_v}^*(S_\nu) + (\Lambda_{\tau_v} - \Lambda_{\tau_v}^*)(S_\nu) \\ &\quad + 2h\nu^3/c^2 \} e^{-h\nu/kT} d\nu \end{aligned} \quad (2.64)$$

In view of (2.62) and denoting $\Delta J_\nu = (\Lambda_{\tau_v} - \Lambda_{\tau_v}^*)(S_\nu)$

$$\begin{aligned} R_{ij} &= 4\pi \int_c^{\infty} (\sigma_{ij}/h\nu) S_\nu d\nu + 4\pi \int_w^{\infty} (\sigma_{ij}/h\nu) 1/2 S_\nu(\tau_v=\gamma) d\nu \\ &\quad + 4\pi \int_0^{\infty} (\sigma_{ij}/h\nu) \Delta J_\nu d\nu \end{aligned} \quad (2.65)$$

$$\begin{aligned}
R_{ji} = & 4\pi (n_i/n_j)^* \int_c (\sigma_{ij}/h\nu) (S_\nu + 2h\nu^3/c^2) e^{-(h\nu/kT)} d\nu \\
& + 4\pi (n_i/n_j)^* \int_w (\sigma_{ij}/h\nu) (1/2 S_\nu(\tau_\nu=\gamma) + 2h\nu^3/c^2) e^{-(h\nu/kT)} d\nu \\
& + 4\pi (n_i/n_j)^* \int_0^\infty (\sigma_{ij}/h\nu) \Delta J_\nu e^{-(h\nu/kT)} d\nu
\end{aligned} \tag{2.66}$$

where c means integration over all core frequencies, those such that $\tau_\nu \geq \gamma$, and w means integration over all wing frequencies, those with $\tau_\nu < \gamma$. The term ΔJ_ν is called the *correction term* and is calculated from the occupation numbers of the previous iteration (actually a further approximation). The wing terms contain only the source function from deeper layers, which has been calculated already. (Remember that the $\Lambda_{\tau_\nu}^*$ operator is block diagonal). Thus, the only unknown terms are the core integrals, containing the local occupation numbers.

To avoid the non-linearity of these terms we can assume that the source function in the core of the transition $i \leftrightarrow j$ is dominated by these two levels. Under this assumption (DETAILED BALANCING) the downward and upward rates are equal, and the core integrals disappear in (2.65) and (2.66).

Although a linearization might also provide a solution, the detailed balancing hypothesis simplifies the equations and requires less computation time.

The fact that the local occupation numbers are the only unknown variables represents the greatest advantage of the ALI method because only matrices of order $(n_{\text{level}} \times n_{\text{level}})$ have to be inverted. The computing time scales approximately linearly with the number of frequencies because only the integrals of the radiative rates must be calculated.

Now all terms are known and the method can be iterated as follows:

- 1) From the current estimates of the occupation numbers, calculate the optical depth scale and the source function at each depth.
- 2) Perform a formal solution.
- 3) The term $\Delta J_\nu = (\Lambda_{\tau_\nu} - \Lambda_{\tau_\nu}^*)(S_\nu)$ can be calculated from 1) and 2).
- 4) The statistical equilibrium equations are solved, starting at the bottom

of the atmosphere and new occupation numbers are calculated.

5) The whole process is iterated until convergence is achieved.

The ALI method works very well for lines, but for the continuum a lambda iteration is sometimes better conditioned for convergence. Unfortunately, this is only possible when the continuum is optically thin, i.e., when it is formed in regions where the collisions still play an important role in the determination of the corresponding population numbers. When, on the contrary, the continuum is optically thick, instabilities appear in the iteration process. This is probably due to the fact that the core - wing separation (in frequency and in depth) is too crude for the continuum. We must then choose a high value of γ , but this in effect converts the method to a lambda iteration.

If the continuum is extreme optically thick, it is possible to apply the hypothesis of detailed balancing throughout the entire atmosphere. Of course the occupation numbers are then not reliable in the upper layers of the atmosphere but this is not a problem because a) the opacities in the outer layers of our atmospheres models are artificially too low because of the neglect of wind opacities; b) we assume hydrostatic equilibrium in these layers, which does not agree with the observations; and c) we use in our study only lines formed deeper in the atmosphere and that are consequently not affected by this difference in the treatment of the continuum.

However, there are combinations of stellar parameters for which none of the above solutions is adequate. Here we use the modification of the approximate lambda operator given by *Werner* (1986) and *Hamann* (1985). We write for the core

$$\Lambda_{T_v}^*(S_v) = S_v (1 - e^{-\tau_v/\beta}) \quad (2.67)$$

The core integral will again disappear in equation (2.65) under the assumption of detailed balancing, but not in equation (2.66). The remaining term may be written:

$$R_{ji}^c = 4\pi (n_i/n_j)^* \int_c (\sigma_{ij}/h\nu) (2h\nu^3/c^2) e^{-\tau_v/\beta} e^{-(h\nu/kT)} d\nu \quad (2.68)$$

Observe that when $\beta \rightarrow 0$ the ALI method is recovered, and when $\beta \rightarrow \infty$ we obtain the lambda iteration. If β has some finite value greater than zero, the core saturation hypothesis is somewhat relaxed, the lambda iteration approached and the iteration process stabilizes.

CHAPTER III

New H and HeII Line Formation using the ALI Method

We have applied the Accelerated Lambda Iteration (ALI) to line formation problems in H and HeII in model atmospheres that correspond to the stars reviewed in the Introduction (O, sdO, sdB, CPN). In section III.1. the technique is tested. Sections III.2. and III.3. are dedicated to the presentation of the results for H and HeII respectively. We compare them with previous calculations and interpret our findings, and finally we apply them by comparing with observations. In section III.4. we treat for the first time in detail the overlap of H and HeII lines, one of the problems discussed in the Introduction.

III.1. – Test for the Accelerated Lambda Iteration

To test the new technique we try to reproduce some previous standard calculations. We have used the model atmospheres of *Kudritzki* (1976) which have five NLTE levels of Hydrogen plus protons and include as radiative bound – bound transitions only $L_\gamma - \alpha$, $L_\gamma - \beta$, $L_\gamma - \gamma$, H_α , H_β and P_α in the statistical equilibrium equations. The models also include the ground levels of HeI, HeII and HeIII, but we use them only to provide background opacity in our test.

The Accelerated Lambda Iteration has already been tested by *Werner and Husfeld* (1985), so that we only present here some results to demonstrate its main properties.

We set the occupation numbers of Hydrogen to their LTE values and, keeping the temperature – density structure of the models fixed, iterate the populations until their changes are everywhere less than 10^{-3} .

We test first the dependence on the γ – parameter. Table 3.1 contains the results for several different models, and Fig. 3.1 – 3.2 show the convergence for two of these models. The continuum is treated in two different ways: in case a the ALI is used for bound – free transitions as well and in case b only the Λ – iteration

is applied.

From Table 3.1 some conclusions may be drawn:

- a) Too low a value of γ produces divergence.
- b) The value of γ needed to reach convergence increases with decreasing temperature in case a, but remains approximately constant in case b.
- c) The number of iterations needed increases with increasing γ and with decreasing temperature.
- d) It is slightly advantageous to use the Λ - iteration for the continuum.

These points may be explained as follows: Point a) is due to the failure of the core - saturation approximation at transparent frequencies. Point b) reflects the main problem of the ALI: the poor treatment of the energy transfer in the continuum. The profile function of the continuum is much shallower than that of the lines making the distinction between core and wing frequencies more diffuse. Thus a greater value of γ is required to avoid instabilities. Point c) is a consequence of two effects: first, the Λ - iteration is recovered for great values of γ , so that convergence is slower when γ increases; second, when the temperature decreases in the models of Table 3 1, the Hydrogen transitions become optically thicker, and more iterations are needed for the same value of γ Point d) finally is simply the combination of b) and c)

Thus we will use the Λ - iteration for bound - free transitions together with values of γ around 3.

To be sure that the corrections do not stabilize at some small value (as they do in the Λ iteration) we continue the iteration process until a convergence of 10^{-8} is reached. We have performed this test for the models with $T_{\text{eff}} = 75000$ K, $\log g = 5.0$ ($\gamma = 2$) and $T_{\text{eff}} = 40000$ K, $\log g = 4.0$ ($\gamma = 3$) The desired convergence is reached without problem after 35 and 50 iterations respectively.

The time needed for one iteration on a Cyber 175 was always less than 10 seconds. The time needed by the complete linearization method code from Kudritzki (1976) is 180 seconds for the same problem.

Model $T_{\text{eff}}, \log g$	γ	Number of Iterations	
		a	b
75000, 5.0	1.0	Diverges	
	2.0	10	10
	3.0	12	
	4.0	13	13
	7.0	14	
	11.0	15	
50000, 6.5	1.0	Diverges	Diverges
	3.0	13	13
	4.0	14	
	7.0	16	
	11.0	17	
50000, 4.0	3.0	Diverges	14
	5.0	Diverges	17
	6.0	19	
	8.0	20	20
	10.0	21	
40000, 4.0	3.0	Diverges	16
	4.0	18	18
	6.0	22	21
	9.0	25	25

Table 3.1 – Results for tests with different models and γ – parameters. Case a: continuum is treated with ALI; case b: continuum is treated with Λ – iteration.

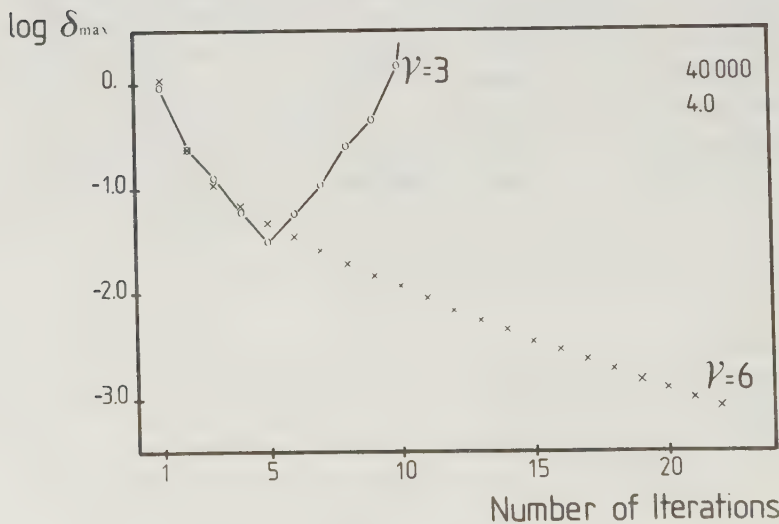
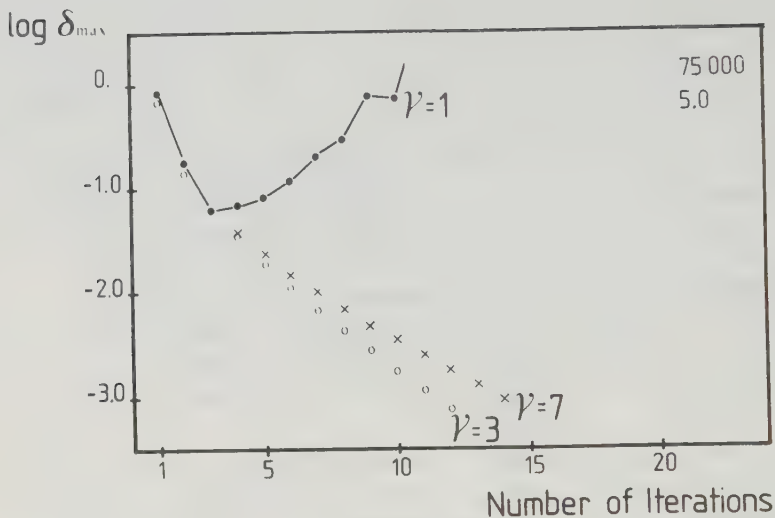


Fig. 3.1 (upper) and 3.2 (lower): Convergence behaviour of the ALI for different γ 's in models with $T_{\text{eff}} = 75000$, $\log g = 5.0$ and $T_{\text{eff}} = 40000$, $\log g = 4.0$. Both models have normal Helium abundance. δ_{max} is the maximum correction to the occupation numbers for all depths.

Finally, a comparison of our tests with those performed by *Werner and Husfeld* (1985) reveals perfect agreement between both sets of calculations.

III.2. - Hydrogen

In this section we present the results of extensive NLTE line formation calculations for Hydrogen using the Accelerated Lambda Iteration. We use a sequence of Hydrogen model atoms with an increasing number of levels and transitions. We start with 5 NLTE levels plus protons, 5 bound - free transitions and 6 lines (with depth - independent Doppler profiles in the statistical equilibrium equations), which lead to complete radiative coupling of the lowest four levels. This corresponds to the older calculations of *Auer and Mihalas* (1972) and *Kudritzki* (1976). We shall refer to them as the *standard calculations* for Hydrogen. (For details such as atomic data and formulae see Appendix). The frequency grid in this case consists of 74 points. The model atmosphere on which all the calculations are based are NLTE H/He models of normal composition ($Y = N(\text{He})/(N(\text{H}) + N(\text{He})) = 0.09$) with 90 depth points (see, for instance, *Kudritzki*, 1976). The most elaborated Hydrogen model atom has 10 NLTE levels plus protons with 10 bound - free transitions and 45 lines (complete radiative coupling of all NLTE levels), with depth - dependent profiles including Doppler and Stark broadening using the theory of *Griem* (1964) as formulated by *Auer and Mihalas* (1972). In this case we use 923 frequency points. The total number of levels is in all cases 16, the remaining upper levels being always treated in LTE. It should be noted that, even at these temperatures (greater than 30000 K) a careful integration of the Balmer continuum must be performed. We use Simpson's rule with five points.

For all Hydrogen calculations described here a convergence of 10^{-4} in the occupation numbers was required.

In section III.2.1. we discuss in detail, for a representative model, the influence of the number of NLTE levels and the broadening mechanism considered in the transfer and statistical equilibrium equations on line profiles and populations. A table with results for other models is then given. In section III.2.2. the new results are compared with the observations showing the improvement represented by our calculations over previous ones.

III.2.1. – Numerical Results

For our discussion we have chosen a model with $T_{\text{eff}} = 60000$ K, $\log g = 5.0$ and normal Helium abundance, $Y = 0.09$. Such a model is representative of many Central Stars of Planetary Nebulae (see *Méndez et al.*, 1985) and is therefore of particular importance for the quantitative spectroscopy of these objects. Other models, that correspond to normal O stars or to O Subdwarfs show qualitatively the same effects and the results are summarised in Table 3.5.

We have tested the model as described in section III.1., and obtain agreement with the previous NLTE occupation numbers of Kudritzki to better than one part in a thousand.

As a first step the fifth level is coupled radiatively with the lower ones by introducing $L_{\gamma} - \delta$, H_{γ} , P_{β} and B_{α} as additional transitions. The changes in the occupation numbers for each depth point (in other figures we will consider only some representative depth points) are plotted in Fig. 3.3. It can be seen that levels 1 to 4 are now more heavily populated and level 5 is depopulated. The explanation is clearly that electrons cascade to lower levels when the new lines become optically thin. The previous populations are maintained for $n = 5$ until the density becomes very small. In the uppermost regions of the atmosphere, recombination dominates and the electrons cascade from level 5 where they had previously been kept artificially.

The effect of these changes on the emergent profiles can be explained as follows. Assuming the Eddington – Barbier relation as our approximation we may write

$$H_{\nu}(0) = 1/4 S_{\nu}(\tau_{\nu} = 2/3) \quad (3.1)$$

If we consider the source function in the line as being the total source function, we can show that

$$S_{\nu}(\text{old})/S_{\nu}(\text{new}) = [\beta(n_i/n_j) - \alpha] / [(n_i/n_j) - \alpha] \quad (3.2)$$

where

$$\beta = 1 + (\delta n_i / n_i) / 1 + (\delta n_j / n_j) \quad (3.3)$$

and

$$a = (n_i / n_j)^* e^{-(h\nu / kT)} \quad (3.4)$$

If we have $\beta > 1$, we obtain $S_{\nu}(\text{old}) > S_{\nu}(\text{new})$ and the new profiles will become deeper. On the other hand, if $\beta < 1$ then $S_{\nu}(\text{old}) < S_{\nu}(\text{new})$ follows and the new profiles become shallower (for both cases $n_i / n_j > g_i / g_j$ was taken into account). In Table 3.2 we have summarized the possibilities that can lead to the different cases.

δn_j δn_i Positive Negative Positive $\delta n_i / n_i > \delta n_j / n_j \rightarrow \beta > 1$ $\delta n_i / n_i < \delta n_j / n_j \rightarrow \beta < 1$ $\beta < 1$ Negative $\beta > 1$ $\delta n_i / n_i < \delta n_j / n_j \rightarrow \beta > 1$ $\delta n_i / n_i > \delta n_j / n_j \rightarrow \beta < 1$	
--	--

Table 3.2 - The possible values of β in expression (3.2)

As can be seen all the lines including $n = 5$ will have deeper cores. Lines such as H_{β} where both levels are now repopulated will become deeper or shallower depending on the relative changes of each level. Looking at Fig. 3.3 we see that H_{β} must become deeper, because $\delta n_i > 0$ and $\delta n_j \approx 0$ in the region of formation.

Table 3.3 gives the results of the final profile calculations and shows that in fact the cores of both H_{β} and H_{γ} become deeper when all radiative transitions up to $n = 5$ are included.

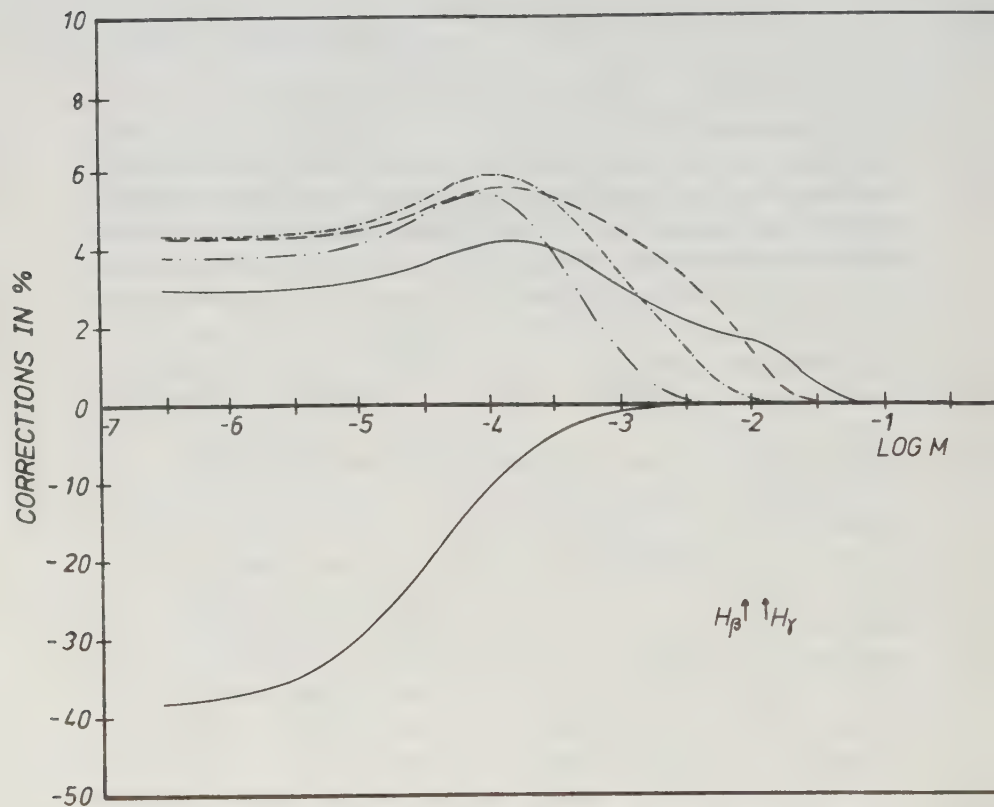


Fig. 3.3: Percentage changes in the occupation numbers of the five lower levels of Hydrogen versus depth in the atmosphere (logarithm of the mass scale) after introduction of the lines belonging to $n=5$ with depth-constant Doppler broadening. Note that the negative scale is five times greater than the positive one. Arrows indicate the point of the atmosphere in which the opacity in the centre of H_γ and H_β reaches $2/3$. Full drawn: $n=1$ (positive) and $n=5$ (negative); (— —): $n=2$; (- · -): $n=3$; (- · · -): $n=4$.

line	$\Delta\lambda$		$\Delta\lambda$		$\Delta\lambda$		$\Delta\lambda$		$\Delta\lambda$	
	0	1	0	1	0	1	0	1	0	1
H β	3.7	0.9	3.4	2.1	5.1	2.0	0.1	0.5	11.9	5.6
H γ	2.5	0.4	3.1	1.3	4.0	1.1	0.3	0.5	9.5	3.3

Table 3.3 - Percentage changes in the residual fluxes of H β and H γ at $\Delta\lambda = 0$ and 1Å. The changes are always relative to the previous columns and are in the same direction. Columns 1-2: adding the lines belonging to $n=5$; columns 3-4: including Stark broadening (with all lines between levels 1 and 5); columns 5-6: including levels 6-10 and their lines with Doppler broadening; columns 7-8: including Stark broadening for lines belonging to levels 6-7; columns 9-10: total effect.

Until now we have performed the calculations with depth-independent Doppler profiles. Now we introduce Stark broadening throughout the entire atmosphere. Although in the above formulation of the ALI method (section II.10.) overlapping in the lines was not allowed due to the assumption of detailed balancing, Stark broadening produces very broad lines in hot stars, that may then overlap. We relax this assumption somewhat by writing the contribution from the $i \leftrightarrow j$ transition explicitly and group all others together in the source function

$$S_v = [(\epsilon_v^{ij} + \epsilon_v^{ov}) / (\chi_v^{ij} + \chi_v^{ov})] \quad (3.5)$$

here ϵ_v^{ij} , χ_v^{ij} are the line emission and absorption coefficients of the transition $i \leftrightarrow j$, whereas ϵ_v^{ov} , χ_v^{ov} are the same quantities for the overlapping lines. The core radiative rates then consist of two terms

$$\begin{aligned} R_{ij}^c = & 4\pi \int_c \chi_v^{ij} / (\chi_v^{ij} + \chi_v^{ov}) (\sigma_{ij}/h\nu) (\epsilon_v^{ij} / \chi_v^{ij}) dv \\ & + 4\pi \int_c \chi_v^{ov} / (\chi_v^{ij} + \chi_v^{ov}) (\sigma_{ij}/h\nu) (\epsilon_v^{ov} / \chi_v^{ov}) dv \end{aligned} \quad (3.6)$$

$$\begin{aligned}
R_{ji}^c = & 4\pi(n_i/n_j)^* \int_c \chi_v^{ij} / (\chi_v^{ij} + \chi_v^{ov}) (\sigma_{ij}/h\nu) \{ (\epsilon_v^{ij}/\chi_v^{ij}) + (2h\nu^3/c^2) \} e^{-(h\nu/kT)} d\nu \\
& + 4\pi(n_i/n_j)^* \int_c \chi_v^{ov} / (\chi_v^{ij} + \chi_v^{ov}) (\sigma_{ij}/h\nu) \{ (\epsilon_v^{ov}/\chi_v^{ov}) + (2h\nu^3/c^2) \} \\
& \times e^{-(h\nu/kT)} d\nu
\end{aligned} \tag{3.7}$$

Now the first terms of R_{ij}^c , R_{ji}^c again cancel in the rate equations as in (2.65) and (2.66), but the second terms remain as correcting *overlapping terms* in the algorithm, and they are calculated from the previous iteration cycle.

The changes in the occupation numbers to be added to those of Fig. 3.3 are plotted in Fig. 3.4. They are very small in the outer layers but become larger for $n=2,3$ in the line formation region. Columns 3-4 of Table 3.3 show that the effect is also present outside the actual core, for instance at $\Delta\lambda = 1\text{\AA}$. The new profiles are again deeper for the reasons described earlier and summarised in Table 3.2.

To explain the changes in the occupation numbers, we must distinguish between the two effects we have introduced with the Stark broadening, depth dependent profiles and Stark wings. For this purpose, we have repeated our calculation in two steps: first, we introduce depth dependent Doppler profiles and then Stark profiles. The result is plotted in Fig. 3.5 for $n=1$ and $n=2$ and demonstrates that the depth dependence of the Doppler profiles is of no importance. The changes of $n=1$ at $\log m \approx -1.0$ and $n=2$ at $\log m \approx -2.0$ must be explained by the Stark wings.

The wings of the Lyman lines are formed deep in the atmosphere (for example, for $L_y - a$ the point at $-3\Delta\nu_D$ from the center reaches $\tau_v \approx 2/3$ at $\log m \approx -0.8$). Then, because of the complete redistribution assumption, exciting photons previously trapped in the core now have a chance to escape so that more electrons stay in the ground state, populating it and depopulating the others. But for these upper levels, collisions and bound-free transitions dominate at these depths so that they maintain their previous populations.

The above mechanism is effective only if the former Doppler core is completely optically thick. When part of the Doppler core becomes optically thin, the photons have a chance to escape in both cases (with only Doppler profiles and with

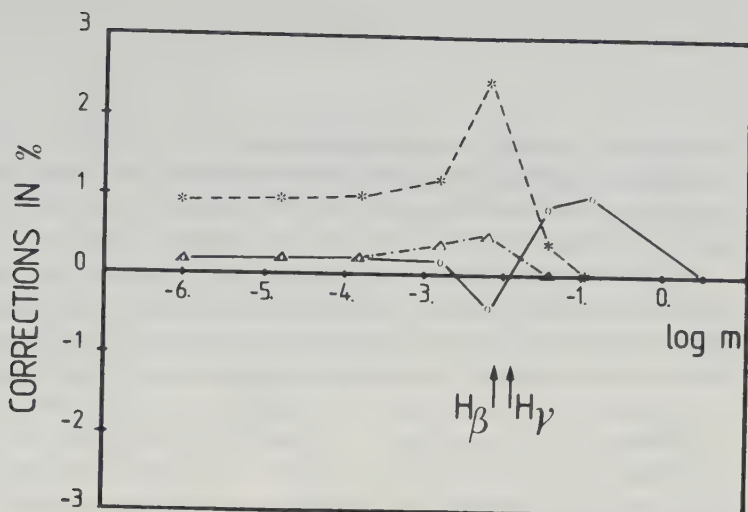


Fig. 3.4: Percentage changes in the occupation numbers of the three lower levels of Hydrogen, to be added to those of Fig. 3.3, versus logarithm of the mass scale for some representative depth points after introduction of the Stark broadening for all lines coupling levels 1 to 5. Full drawn lines: $n = 1$; (- -): $n = 2$; (- · -): $n = 3$.

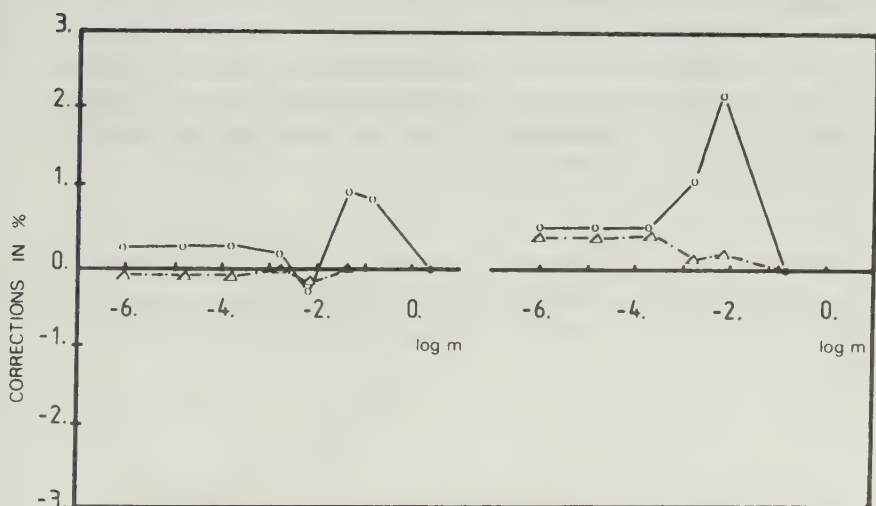


Fig. 3.5 : Percentage changes in the occupation numbers of level 1 (left) and 2 (right) of Hydrogen. (- · -): changes when depth - dependent Doppler broadening is considered relative to the depth independent one. Full drawn: changes when Stark profiles are considered, relative to depth - dependent Doppler profiles. Both effects together give the changes plotted in Fig. 3.4. Only some representative depth points are shown.

Stark profiles). However, we now have more opacity in the wings due to the Stark broadening so that even more exciting photons are trapped. As a consequence, the upper level is populated and the lower one is depopulated.

The assumption of complete redistribution can be considered correct in the core (*Mihalas*, 1978, Chap.13). A failure of this assumption in the wings (which would not be complete), would only allow additional photons to escape, reinforcing – probably only slightly – the effect described here.

Adding now the levels from 6 to 10 and their lines (with only Doppler broadening), we obtain the same effect as when we included the lines of level five: lower levels are repopulated and upper ones are depopulated. Columns 5 – 6 of Table 3.3 contain the effect on the emergent profiles of H_{β} and H_{γ} .

Finally, we introduce the Stark profiles for lines belonging to levels 6 and 7. The changes are very small as can be seen from columns 7 – 8 of Table 3.3. We conclude that it is not necessary to include the Stark broadening of the lines belonging to levels 8, 9 and 10.

To ensure that it is not necessary to include levels higher than $n = 10$, we made a test by adding levels one at a time (including Stark broadening too). The result is shown in Table 3.4. The changes in the emergent profiles after the inclusion of level 10 are everywhere smaller than 0.5% We conclude that no more levels are needed.

Number of levels	H_{β}			H_{γ}		
	$\Delta\lambda = 0$	$\Delta\lambda = 1$	$\Delta\lambda = 2$	$\Delta\lambda = 0$	$\Delta\lambda = 1$	$\Delta\lambda = 2$
6	3.2	1.0	0.5	1.7	0.6	0.2
7	1.3	0.7	0.3	1.2	0.5	0.2
8	0.9	0.5	0.3	0.7	0.4	0.2
9	0.4	0.4	0.1	0.4	0.3	0.1
10	0.3	0.1	0.1	0.3	0.1	0.1

Table 3.4 – Percentage changes in the residual fluxes of H_{β} and H_{γ} at $\Delta\lambda = 0, 1$ and $2 \text{ \AA}$ when levels 6 to 10 and their lines (including Stark broadening) are considered. Changes are always relative to the previous row and are in the same direction (profiles become deeper).

The total effect relative to the *standard* calculations for the emergent profile of H_β is 12% ($\Delta\lambda = 0\text{\AA}$), 5.5% ($\Delta\lambda = 1$) and 2% ($\Delta\lambda = 2$), and for H_γ 9.5%, 3.5% and 1%, respectively. In all cases the new profiles are deeper. Table 3.5 contains the results for other models. As can be seen, the effect is present at all temperatures and gravities.

The step - by - step improvements in the statistical equilibrium calculations lead to changes that are small at each stage, but since they are always in the same direction, they produce an observable effect, as we will show in the next section.

Model	$\Delta\lambda =$	H_β			H_γ		
		0	1	2	0	1	2
33000,4.15,0.10		15.0	3.5	1.5	14.0	3.0	1.0
40000,4.00,0.09		13.5	3.0	1.0	13.0	2.0	1.0
50000,4.00,0.09		12.0	3.0	0.	12.5	2.0	0.
50000,5.00,0.09		12.5	5.0	1.5	10.0	3.5	1.0
50000,6.50,0.09		8.0	4.0	2.0	4.5	2.5	1.5
51000,4.50,0.09		12.0	4.5	1.0	11.0	2.5	1.0
60000,5.25,0.09		11.5	5.5	2.0	9.0	3.5	1.0
60000,5.00,0.09		12.0	5.5	2.0	9.5	3.5	1.0
65000,5.30,0.09		10.5	5.0	2.0	8.0	3.5	1.5
75000,5.00,0.09		11.0	6.5	2.0	9.0	4.0	1.5
75000,5.50,0.09		10.5	6.0	2.5	7.0	4.0	1.5

Table 3.5 - Total changes in the residual intensities for several models. Given are effective temperature, $\log g$ and Y . The $\Delta\lambda$ are given in $\text{\AA}$ and the changes in %. All profiles are deeper in our calculations.

III.2.2. – Comparison with the Observations

As was pointed out in the Introduction, observed Balmer line profiles of hot stars have systematically deeper cores than the calculated ones when the star rotates slowly.

We want to show here that the discrepancy disappears if we use our new extended calculations (more levels and Stark broadening included in the statistical equilibrium equations) described in the preceding section. Moreover, because we find the effect in all our models, we conclude that it is masked by rotation in rapidly rotating stars.

We will show that the effect is of special importance for the quantitative spectroscopy of CPN.

For the comparison we use the line formation code of *Simon* (1982) for Helium and for the formal solution. In this code the more realistic theory of *Vidal et al.* (1973) is used for Stark broadening.

Our first example is the sharp lined O9V star τ Sco. It has been analyzed on the basis of *standard* NLTE model atmospheres by *Auer and Mihalas* (1972), who found $T_{\text{eff}} = 31500$ K, $\log g = 4.15$ and $Y = 0.09$. *Schönberner et al.* (1986) in their study of nitrogen rich O stars used τ Sco as a comparison object for differential spectroscopy. From their new observational data (still photographic plates) and *standard* NLTE models they obtained $T_{\text{eff}} = 33000$ K, $\log g = 4.15$ and $Y = 0.1$. In both cases T_{eff} has been determined from the NLTE HeII/HeI ionization equilibrium, whereas $\log g$ followed from the far wings of the Balmer lines. Thus the central parts of the Balmer lines can be used to test the accuracy of the Hydrogen equilibrium calculations. For both temperatures the *standard* calculations do not fit the observed cores of H_{γ} and H_{β} (the hotter temperature being slightly worse). Fig. 3.6a,b and 3.7a,b show high resolution, high S/N line profiles for H_{β} and H_{γ} in τ Sco, obtained by P.E. Nissen (Aarhus) using the CASPEC spectrograph plus CCD attached to the ESO 3.6 m telescope (for details of the observations see *Gehren et al.*, 1985). The failure of the *standard* calculations is obvious from the figures. The improved calculations, however, fit almost perfectly.

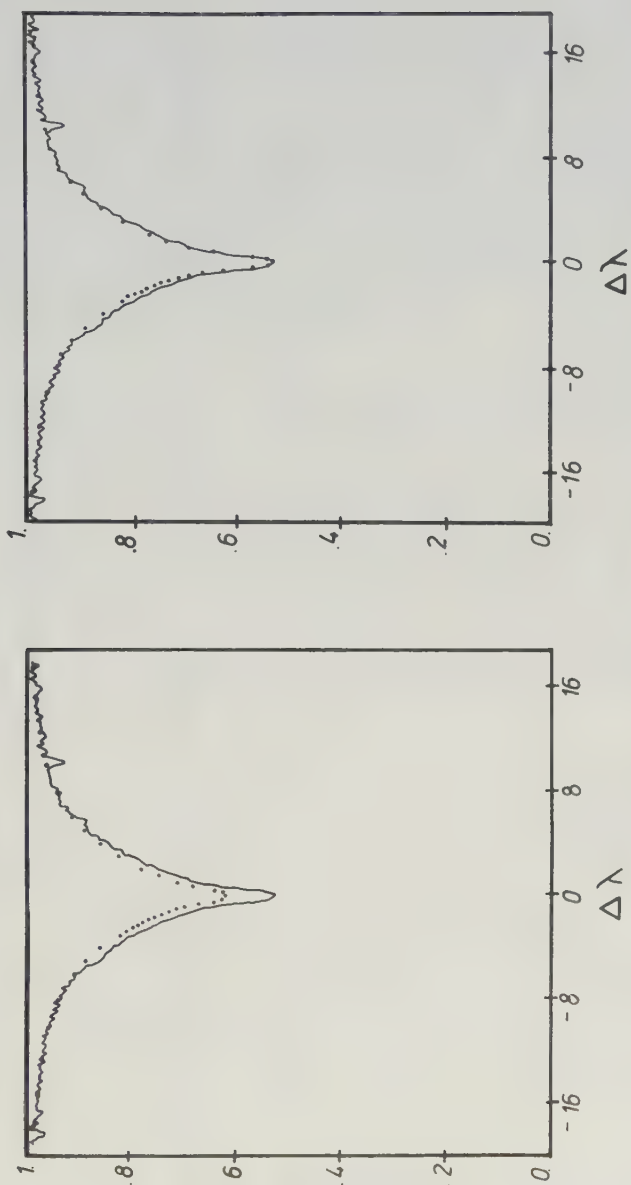


Fig. 3.6a and 3.6b: Fit to the $H\beta$ profile of τ Sco ($T_{\text{eff}} = 33000$, $\log g = 4.15$, $Y = 0.10$) using the *standard* calculations (left) and our calculations (right).

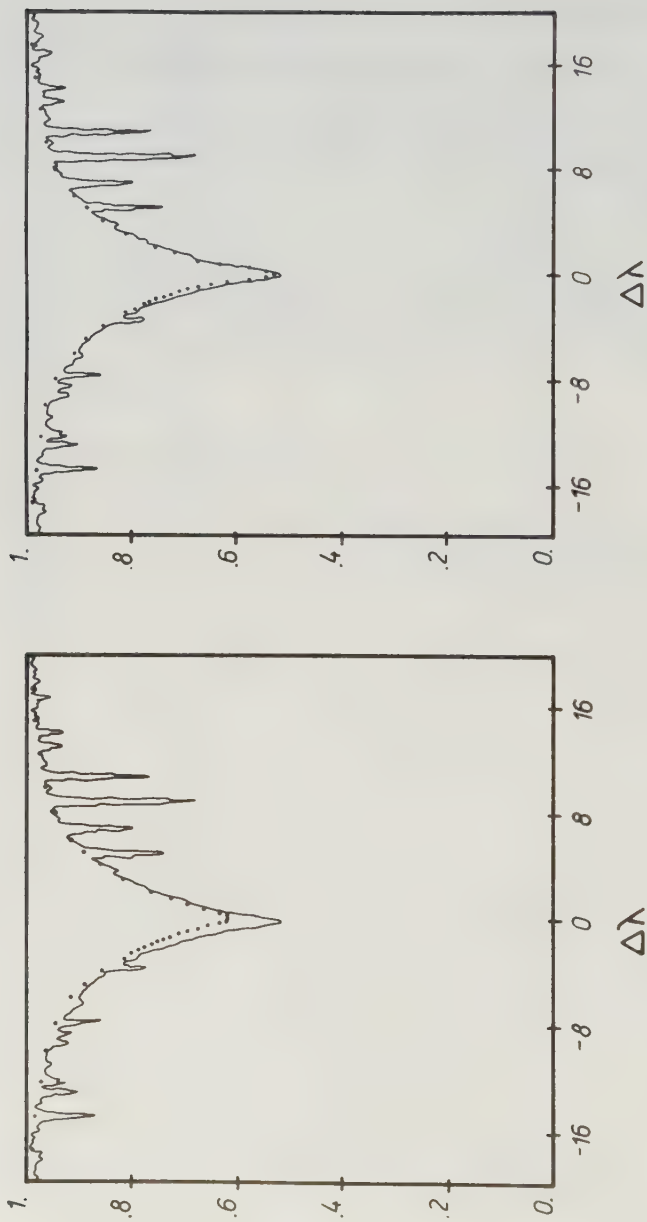


Fig. 3.7a and 3.7b: Same as the Fig. 3.6a and 3.6b for H γ

The second example is ROB 162, a 13^{th} -magnitude sdO star (probably a CPN) in the globular cluster NGC 6397. This object has been studied very recently by *Heber and Kudritzki* (1986) who also took CASPEC spectra of this rather faint object. The corresponding profiles of H_{γ} and H_{δ} are shown in Fig. 3.8 and 3.9. The stellar parameters of ROB 162 according to Heber and Kudritzki, who again used the HeII/HeI ionization equilibrium and the wings of the Balmer lines in their analysis are $T_{\text{eff}} = 51000$ K, $\log g = 4.5$ and $Y = 0.09$. Fig. 3.8 shows again that the *standard* theory fails in the line core, whereas our new calculations lead to much better agreement.

Our last example is the Central Star of the Planetary Nebula NGC 1360. The NLTE analysis of this object has been carried out by *Méndez et al.* (1981, 1983, 1985), who obtained $T_{\text{eff}} = 60000 \pm {}^{15000}_{5000}$ K , $\log g = 5.2 \pm 0.3$ and $Y = 0.05 \pm 0.02$. The rather large error in T_{eff} is caused by the absence of neutral Helium lines in the spectrum of NGC 1360 so that the Helium ionization equilibrium could not be used. Instead, Méndez et al. had to use the total shape of the Balmer line profiles (core and far wings) to determine T_{eff} and $\log g$. The result was somewhat unsatisfactory. The absence of HeI $\lambda 4471$ indicated $T_{\text{eff}} > 60000$ K, whereas the Balmer lines pointed to $T_{\text{eff}} \leq 60000$ K. Consequently, the adopted value was 60000 K with a large error. This discrepancy has already been mentioned in I.4.

Fig. 3.10 show the H_{γ} profile of NGC 1360 as calculated with the parameters from *Méndez et al.* (1985) (except for the Helium abundance, which does not affect the Balmer profiles here). The calculations for $T_{\text{eff}} = 60000$ K using the *standard* theory and our improvements indicate that now a larger T_{eff} can be fitted by means of the new calculations, since the theoretical cores are still too deep at this temperature. A good fit is obtained at 75000 K which completely resolves the discrepancy discussed above and agrees much better with the UV energy distribution and Zanstra temperature of this Central Star (see *Clegg and Seaton*, 1983). We therefore conclude that for most of the Central Stars analyzed by Méndez et al. the T_{eff} scale will have to be revised towards higher values.

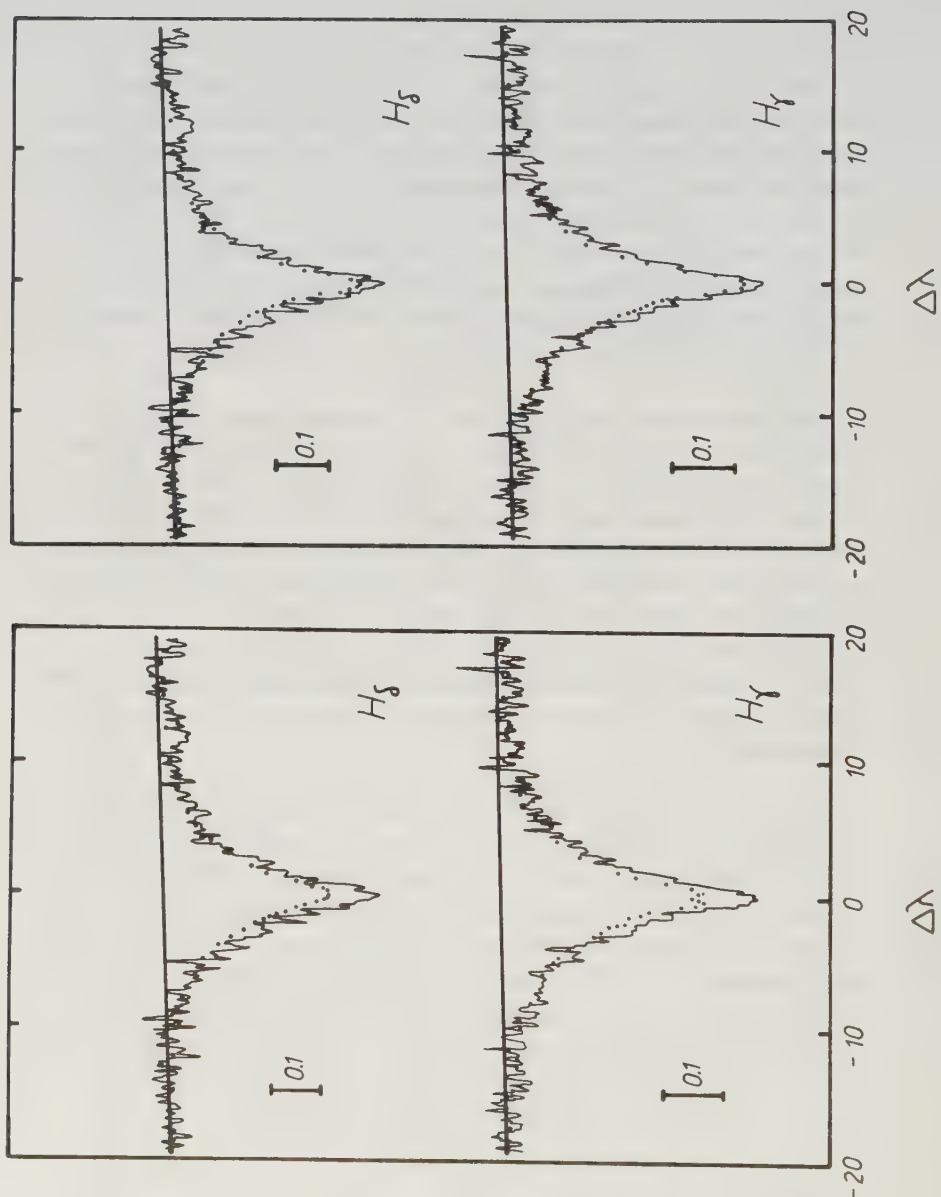


Fig. 3.8 and 3.9: Fit to the H_γ and H_δ profiles of ROB 162 ($T_{\text{eff}} = 51000$, $\log g = 4.5$, $Y = 0.09$) using the *standard* calculations (left) and our calculations (right).

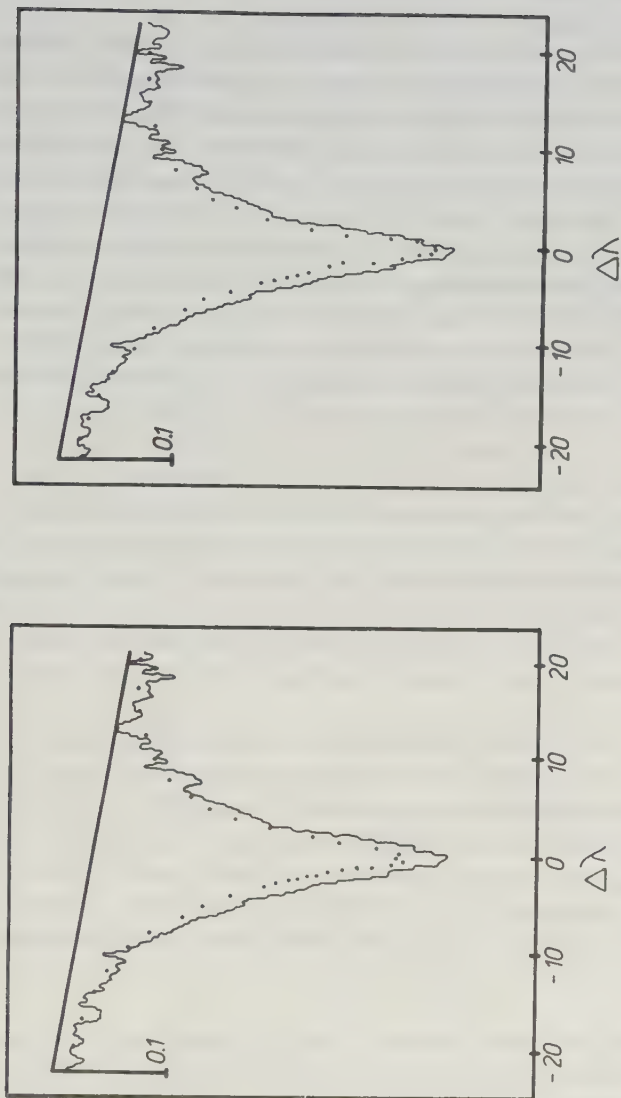


Fig 3.10: Fit to the H γ profile of NGC 1360 after Méndez et al. (1985) (left; standard calculations with $T_{\text{eff}} = 60000$, $\log g = 5.25$, $Y = 0.09$) and after our calculations (right; new parameters are $T_{\text{eff}} = 75000$, $\log g = 5.5$, $Y = 0.09$).

III.3. – Ionized Helium

Extensive NLTE calculations have also been performed for HeII in a similar way as for the Hydrogen calculations. Our initial HeII model has 10 NLTE levels coupled by all radiative and collisional transitions. For the lines, only Doppler broadening is considered in the statistical equilibrium. Levels up to $n = 32$ are assumed to be in LTE with respect to HeIII. This is represented by one NLTE level, as is HeI. The ground levels of consecutive ionization stages are connected by bound – free transitions (again radiatively and collisionally). This corresponds essentially to the *standard* calculations of *Auer and Mihalas* (1972) and *Kudritzki and Simon* (1978) except for the atomic model for HeI. Nevertheless, our coarse treatment of HeI will not affect the results: at our temperatures ($T_{\text{eff}} \geq 30000 \text{ K}$) HeI can be considered a trace element. Consideration of the HeII/HeI ionization balance is then enough to obtain accurate results for the HeII line formation problem.

Our frequency grid has in this case 243 frequency points (not all transitions are linearized in the *standard* calculations). The model atmospheres are the same as for the Hydrogen calculations, except for the extreme Helium rich models ($Y = 0.99$) from *Husfeld* (1986). These models include 5 and 10 NLTE levels for HeI and HeII respectively. The whole collisional coupling and all bound – free radiative transitions are considered but not the bound – bound radiative transitions.

Our most elaborate HeII model atom has 14 NLTE levels, coupled by 91 radiative bound – bound transitions. However, the resonance lines will be kept in detailed balance through the whole calculations, so that only 78 lines are explicitly treated (this approximation will be justified later). Lines connecting levels $n_{\text{low}} \leftrightarrow n_{\text{upper}}$, with $n_{\text{upper}} \leq 7$, are treated with Stark broadening, again using the *Auer and Mihalas* (1972) formulation of the *Griem* (1964) theory. For the rest of the lines we use only Doppler broadening. The total number of frequency points is 655.

The ground level continuum of HeII is usually optically thick. For this reason, it will not be dealt with in the same way as the Lyman continuum of Hydrogen. Instead, we use the β parameter as introduced in expression (2.67) or keep this transition in detailed balance. Again, this last assumption will be justified later.

The other continua of He were treated with the Λ iteration as instabilities may appear when using the ALI, especially in the HeI continuum. The reason is probably that due to the lack of thermal opacity in the far UV, the continuum is formed in deep layers where electron scattering dominates. As a consequence, the hypothesis that the total source function equals the thermal one fails dramatically and introduces large errors. Fortunately, collisions dominate the total rates in these layers, so that the Λ iteration can be used.

For the Helium calculations, convergence is somewhat slower than for Hydrogen (both because γ is slightly greater and the ground level continuum must be treated with the formula (2.67)). Convergence to only the 10^{-3} level is then required in order to save computing time. A test made with $T_{\text{eff}} = 38000$ K, $\log g = 4.25$ and $Y = 0.09$ shows the usual behaviour to a convergence of 10^{-4} .

We start by comparing our results with previous ones in section III.3.1. (for Hydrogen this comparison was already performed in the tests of the ALI method). We justify then the assumption of detailed balancing (III.3.2.), describe the effects of introducing more levels and the Stark broadening in the statistical equilibrium equations (III.3.3.) and compare finally with the observations (III.3.4.)

III.3.1. – Comparison with Previous Results

To perform our comparison we have chosen a model from *Husfeld* (1986) with $T_{\text{eff}} = 75000$ K, $\log g = 5.0$ and $Y = 0.99$. Although this model lies at the upper end of our temperature scale, it does not represent an extreme case. As we shall see later, the ground level continuum of HeII can be treated in detailed balancing, at least in those extreme Helium rich models with $T_{\text{eff}} \leq 50000$ K. In our test model this continuum is still optically thick, but it is not possible to set it in detailed balancing. The high Helium abundance of the model guarantees that Hydrogen has no influence on our results.

Two different tests are made. In the first we try to reproduce *Husfeld's* occupation numbers. Because he only includes collisional and bound – free radiative transitions in his models, we perform a second test by comparing our results with those of a standard program where lines are included.

To reproduce the initial values from Husfeld we proceed in the same way as for Hydrogen: we set the occupation numbers to their LTE values and solve the line formation problem keeping the density and temperature structures fixed.

Due to the high bound - free opacity of the HeII ground level the convergence for the chosen parameters ($\gamma = 5$, $\beta = 10$) is slower than for Hydrogen. To be sure that our corrections do not behave as a Λ iteration, we perform a Λ iteration for all continua (remember that no lines are present).

Fig. 3.11 shows the result. It can be seen that the corrections of the Λ iteration stabilize, whereas the corrections of the ALI method decrease monotonically.

The test has also been used to test the program. Our occupation numbers deviate from those of Husfeld everywhere by less than 1% after 75 iterations.

Because of the lack of bound-bound transitions in Husfeld's models we perform a comparison with DETAIL (Giddings, 1981), another line formation code. In both cases we start with the model from Husfeld and solve again the line formation problem, now introducing the lines connecting levels 2 - 10, allowing for Doppler broadening (the resonance lines are kept in detailed balancing, see next section). The logarithm of the departure coefficients are represented in Fig. 3.12 against the logarithmic mass scale. The differences are surprisingly small, considering the differences between both codes:

- 1) DETAIL uses the complete linearization method in the formulation of Auer and Heasley (1976).
- 2) DETAIL uses 50 depth points, equidistant in $\log m$. Our program uses 90 depth points with a larger spacing in $\log m$ in the outer layers and a shorter one in the line formation region.
- 3) Both codes are absolutely independent and use independent sets of atomic data and formulae.

For the final formal solution we use here the programs SURFACE and ANALYS from Giddings (1981).

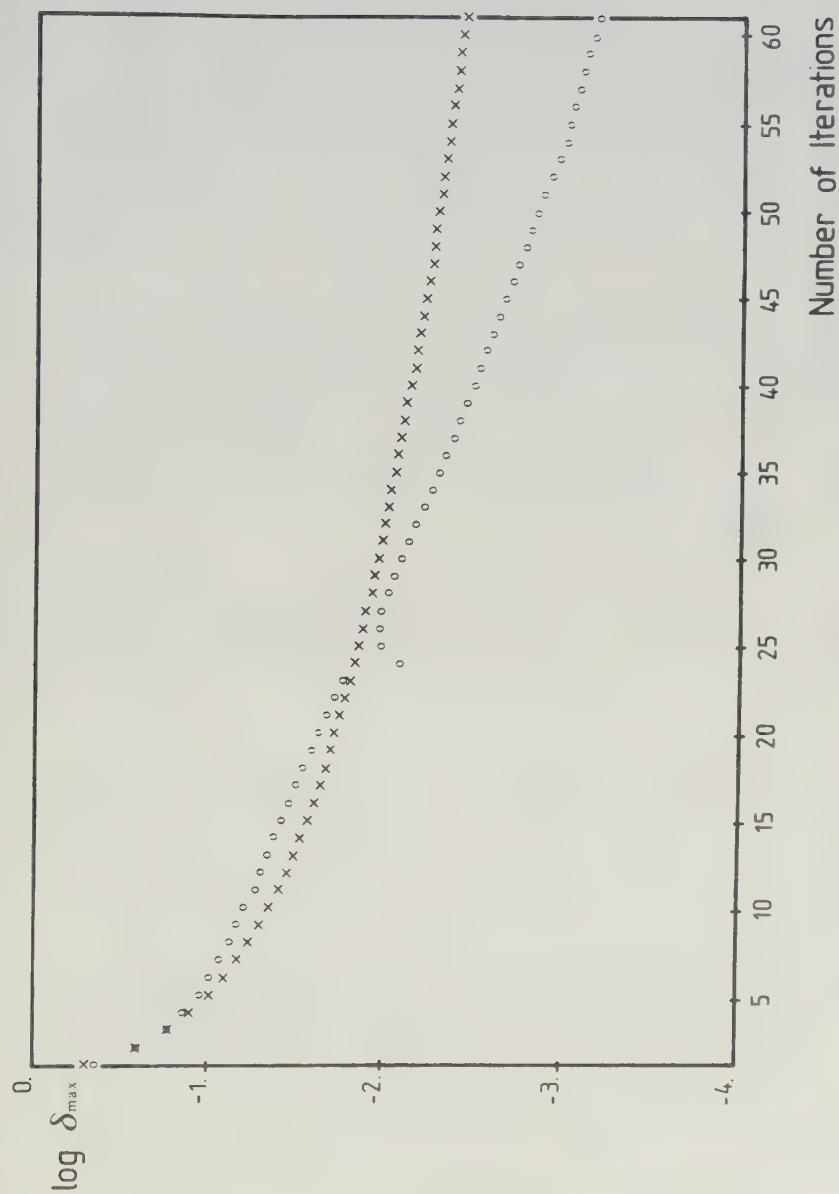


Fig. 3.11: Convergence behaviour of the ALLI (circles) and the Lambda Iteration (crosses) for continuum transitions of Helium in a model with $T_{\text{eff}} = 75000$, $\log g = 5.5$ and $Y = 0.99$. The parameters of the ALLI are $\gamma = 5$, $\beta = 10$. $\delta_{\max}$ are maximum corrections to the occupation numbers for all depths.

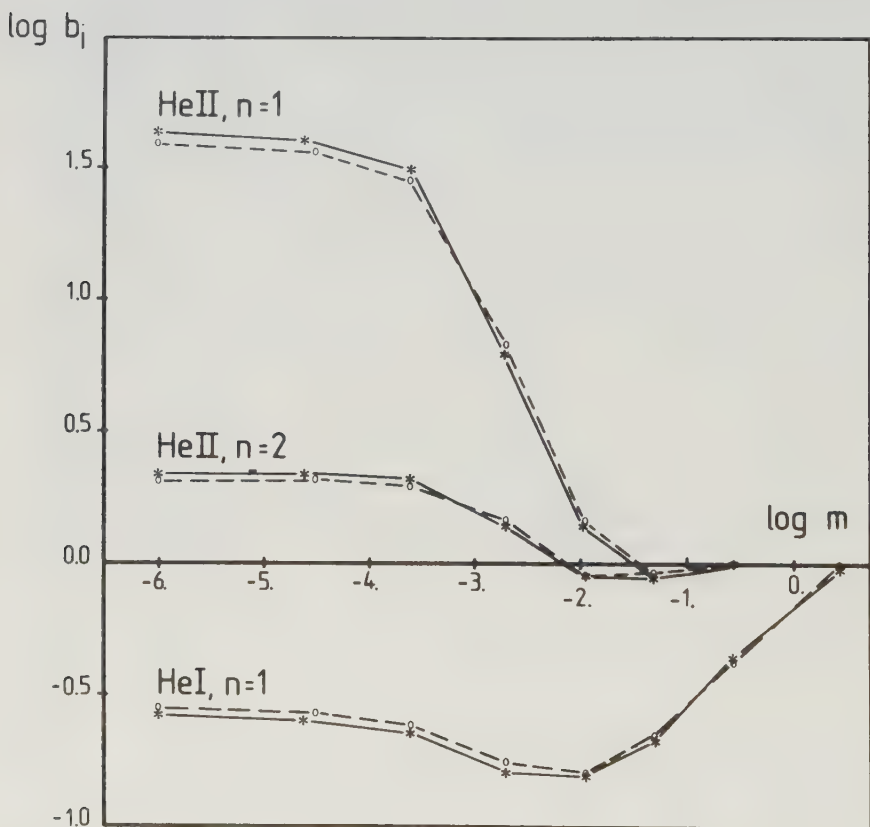


Fig. 3.12: The logarithm of the departure coefficients of the lower levels of HeI and HeII versus the logarithmic mass scale obtained with DETAIL (circles) and with our program (asterisks). Differences become smaller when higher levels are considered. Only some representative depth points are shown.

III.3.2. - The Assumption of Detailed Balancing

The continuum of the ground level of HeII cannot be treated with a Λ iteration due to its great opacity (see Fig. 3.11). The distinction between wing and core photons is not as clear here as in the lines so that the factor $(1 - e^{-\tau \sqrt{\nu/\beta}})$ (see formula 2.67) should be introduced to avoid instabilities. However, this factor resembles the Λ iteration and for very thick continua even small values of β produce a convergence behaviour like that of a Λ iteration.

On the other hand, transitions which are extremely optically thick are formed only in the outer layers of our atmosphere models. Here the models are unrealistic because of the assumption of hydrostatic equilibrium and the lack of line blanketing and wind opacity. For these reasons the assumption of detailed balancing in these layers is of no importance if we can show that the occupation numbers in the regions where the lines of interest are formed are not affected, or that the changes are small enough that the lines themselves remain unchanged.

We wish to show first that the resonance lines of HeII can be kept in detailed balancing for all our model atmospheres. We consider the model with $T_{\text{eff}} = 75000$ K, $\log g = 5.5$ and $Y = 0.09$. In this model the resonance lines will be more transparent than in the other models considered in our calculations, because of the high temperature and the normal Helium abundance

Fig. 3.13 - 3.16 show the departure coefficients of the four lowest levels of HeII against the logarithmic mass scale. It is clear from the figures that the visual profiles will be not affected by the setting of the resonance lines in detailed balancing. Inspection of the profiles confirms this.

For the ground level continuum, tests are made for the models with $T_{\text{eff}} = 50000$ K, $\log g = 5.0$, $Y = 0.99$ and $T_{\text{eff}} = 38000$ K, $\log g = 4.25$, $Y = 0.09$ (corresponding to the star 10 Lac). These models have been chosen because the convergence becomes very problematic when the temperatures are lower.

For 10 Lac, the departure coefficients of the two lower levels of HeII with and without detailed balancing in the continuum are plotted in Fig. 3.17 and 3.18. Lines in the visible (and also the UV line connecting levels 2 and 3 at $\lambda 1640$) are not affected.

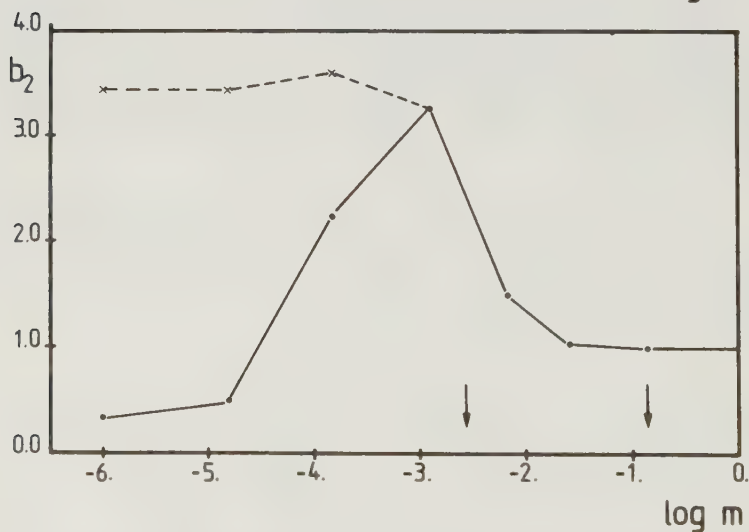
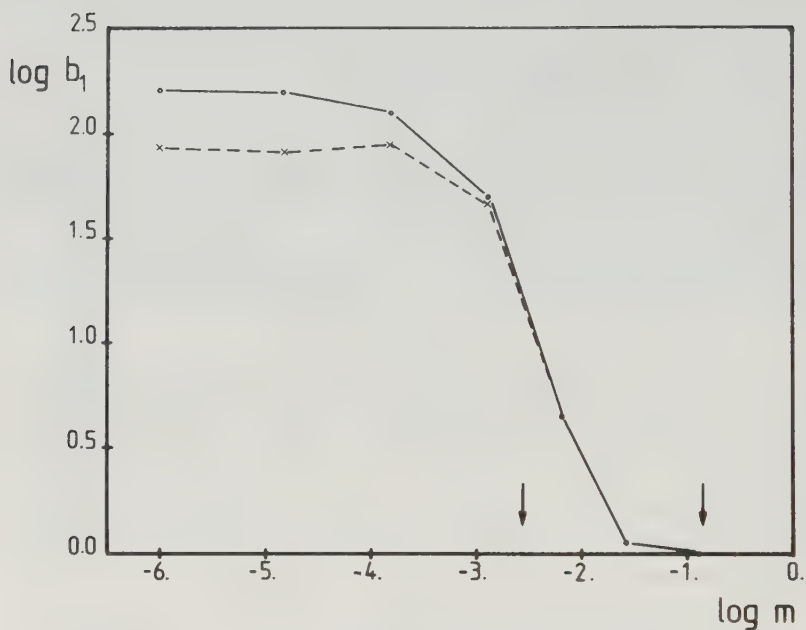


Fig. 3.13 (upper) and 3.14 (lower): The departure coefficients of the ground level (logarithmic) and the second level of HeII versus the logarithmic mass scale for a model with $T_{\text{eff}} = 75000$, $\log g = 5.5$ and $Y = 0.09$. Full drawn: resonance lines not in detailed balancing. (—): resonance lines in detailed balancing. Arrows indicate the formation region of the series of $n=3$ and $n=4$. Only some representative depth points are shown.

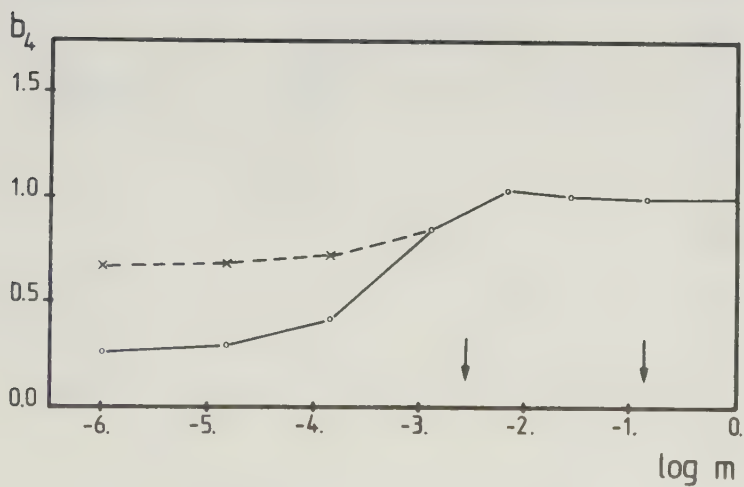
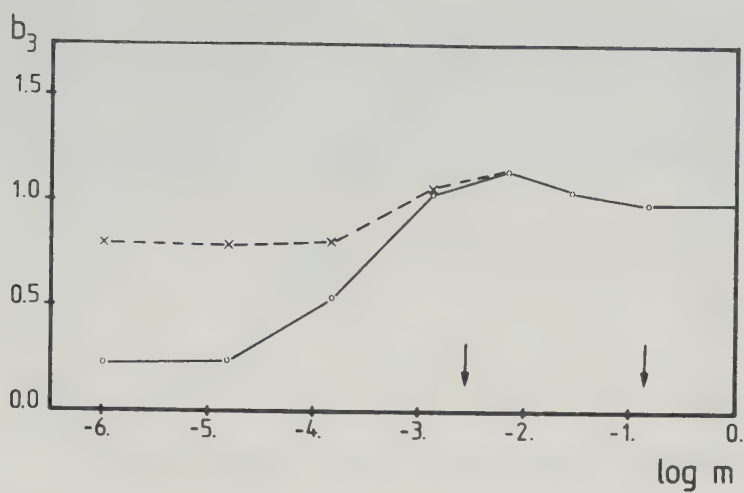


Fig 3.15 (upper) and 3.16 (lower): Same as Fig. 3.14 for $n=3$ and $n=4$.

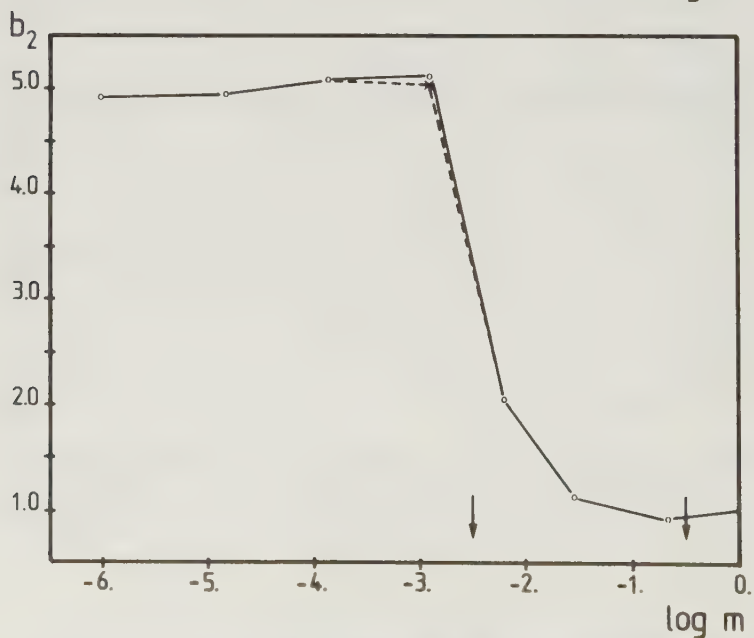
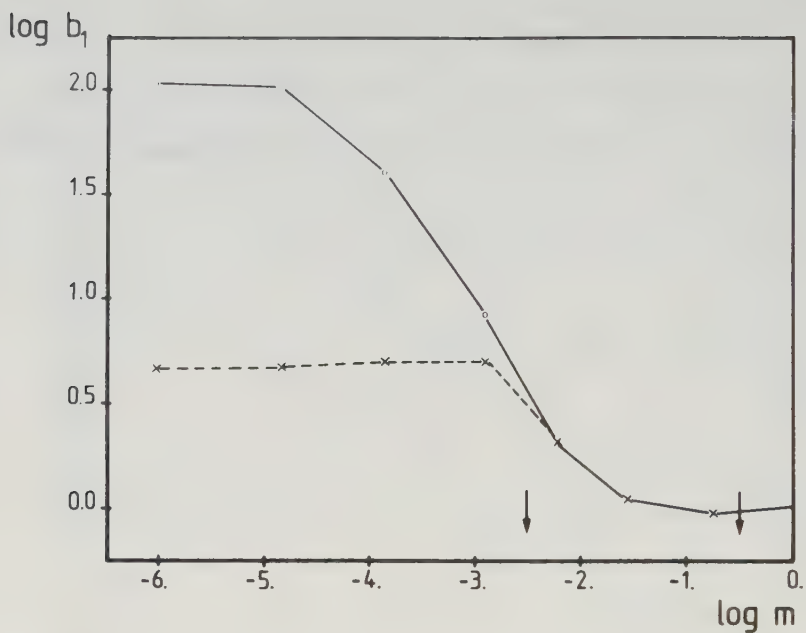


Fig. 3.17 (upper) and 3.18 (lower): Departure coefficients of the first (logarithmic) and second levels of HeII for the model with $T_{\text{eff}} = 38000$, $\log g = 4.25$ and $Y = 0.09$. Full drawn: ground level continuum in detailed balancing; (- -): ground level continuum not in detailed balancing. Arrows indicate the formation region of the series of $n = 3$ and $n = 4$. Only some representative depth points are shown.

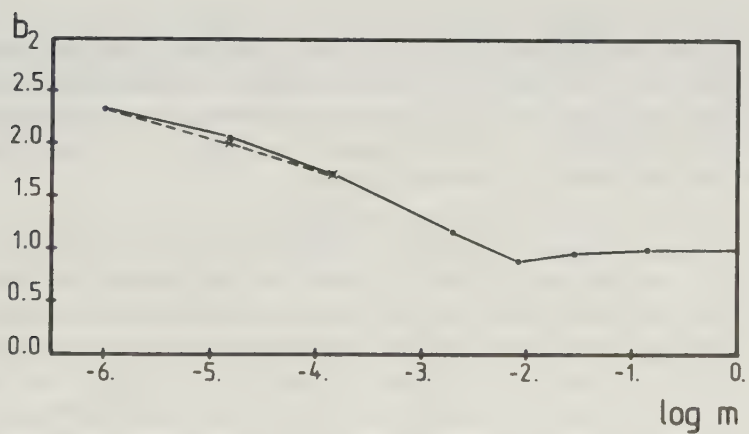
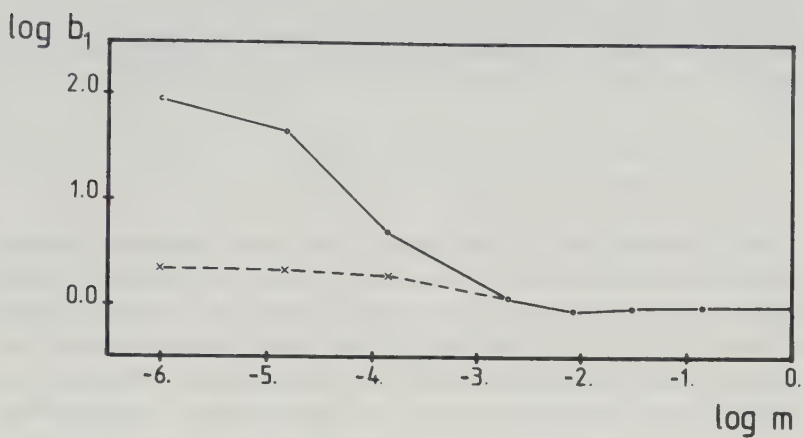


Fig 3.19 (upper) and 3.20 (lower): Same as Fig. 3.17 and 3.18 for the model with $T_{\text{eff}} = 50000$, $\log g = 5.0$ and $Y = 0.99$.

For the Helium rich model the two lower levels are shown in Fig. 3.19 and 3.20. The same comments apply here as for 10 Lac.

We conclude that the assumption of detailed balancing is justified in all three cases.

III.3.3. – Numerical Results

As for Hydrogen, we try to determine the effect of the consideration of Stark broadening and more levels in the calculations. In the case of HeII, however, the *standard* calculations are made with 10 NLTE levels and 45 bound-bound transitions coupling them, although only the most relevant ones are linearized. Next we consider Stark broadening and up to 20 NLTE levels in our calculations, but we study both effects separately, due to the rapid increase in the number of transitions with the number of levels. This separation is possible because the effects are basically independent and add linearly.

In the case of the calculations including Stark broadening the number of levels, transitions and frequencies are similar to those of Hydrogen. When the computations are carried out with 20 NLTE levels and Doppler broadening, 192 transitions are considered from which 171 are lines and the total number of frequency points is 941. In both cases no frequency points are needed for the resonance lines because of the assumption of detailed balancing.

To study the effect of the inclusion of Stark broadening we proceed as follows: starting from the Husfeld model we perform the line formation by assuming Doppler broadening and 10 NLTE levels. This corresponds to the *standard calculations*. Then we consider the Stark broadening for all lines with upper level $n \geq 7$, as for Hydrogen. The other lines are treated only with Doppler broadening. In Table 3.6 we can see the results for our test model with $T_{\text{eff}} = 50000$ K, $\log g = 5.0$ and $Y = 0.99$. For each line, we give the percentage changes in the residual intensity at different $\Delta\lambda$. All the new profiles are now deeper. Only effects greater than 1% are considered.

Line	$\Delta\lambda =$	0.	0.5	1.0	2.0
4 $\leftrightarrow$ 5 ($\lambda 10124$)		1.5	3.0	4.0	3.0
4 $\leftrightarrow$ 7 ($\lambda 5411$)		4.0	3.0	1.5	0.
4 $\leftrightarrow$ 9 ($\lambda 4541$)		2.0	0.	0.	0.
3 $\leftrightarrow$ 4 ($\lambda 4686$)		2.0	3.0	2.5	1.5
3 $\leftrightarrow$ 7 ($\lambda 2511$)		5.0	1.5	0.	0.

Table 3.6 - Percentage changes in the residual intensity of some Helium lines after inclusion of the Stark broadening for lines with upper level $n \leq 7$. New profiles are deeper. The $\Delta\lambda$ are given in Å.

As we can see from Table 3.6, the effect is more important for the lower members of a series, in which it extends to the wings. From the lines usually employed for spectroscopic analyses, transition 4 $\leftrightarrow$ 9 suffers only a very small change, whereas transition 3 $\leftrightarrow$ 4 shows an effect that could be observable in good spectra.

If we add now the Stark broadening for lines with upper level 8, 9 and 10, the changes (to be added to those of Table 3.6) are greater than 1% only for the central point of the transition 4 $\leftrightarrow$ 5. From here, we conclude that the Stark broadening for HeII must be considered, as in Hydrogen, only for lines with upper level $n \leq 7$

The changes in the occupation numbers are formally identical to those of Hydrogen. The only point to bear in mind is that, due to detailed balancing, level $n = 1$ of HeII follows level $n = 2$ and this behaves like level $n = 1$ of Hydrogen.

To study the effect of the upper levels we have divided them into two groups: those with $n = 11$ to $n = 15$ and those from $n = 16$ to $n = 20$.

When we add the first group to our HeII atom description the lower levels are repopulated and the upper ones are strong depopulated in the outer layers and kept in LTE when the density becomes high enough to allow the collisions to dominate again. The interesting effect, as for H, is that there are now channels for the electrons to cascade to the lower levels when the corresponding lines become optically thin.

The effects on the profiles are presented in Table 3.7. Given are the percentage changes in residual intensity, compared with the calculations with 10 levels. As usual, the new profiles are deeper.

As can be seen the effects are small, although they are comparable to the results with Stark broadening for some lines. Consideration of levels 16 – 20 in our models changes the profiles by less than 1% for all frequencies.

	$\Delta\lambda =$	0.	0.5	1.0	2.0
Line					
4 $\leftrightarrow$ 5 ($\lambda 10124$)		2.0	2.0	2.0	1.5
4 $\leftrightarrow$ 7 ($\lambda 5411$)		2.5	1.5	1.0	0.5
4 $\leftrightarrow$ 9 ($\lambda 4541$)		1.5	0.5	0.5	0.
3 $\leftrightarrow$ 4 ($\lambda 4686$)		0.	1.5	1.0	0.5
3 $\leftrightarrow$ 7 ($\lambda 2511$)		2.5	0.5	0.	0.

Table 3.7 – Percentage changes in the residual intensity of some Helium lines after inclusion of levels 11 – 15. New profiles are deeper. The $\Delta\lambda$ are given in Å.

One more test leads us to the final conclusion that the HeII atom is well described by a 14 NLTE level model. This represents 106 transitions, from which 91 are lines (including 13 resonance lines kept in detailed balancing). Stark broadening is considered for transitions with upper level $n \leq 7$. The total number of frequencies in such a model is 655.

In Table 3.8 are given the percentage changes in the residual intensity of several lines between the *standard* calculations and our adopted model with 14 NLTE levels and Stark broadening. Model atmospheres are given by T_{eff} , $\log g$ and Y . The new profiles are always deeper.

Line	4↔5				4↔7				4↔9				3↔4				3↔7			
$\Delta\lambda =$	0	.5	1	2	0	.5	1	2	0	.5	1	2	0	.5	1	2	0	.5	1	2
Model																				
75000,5.50,0.09	3.0	4.0	4.5	4.0	3.0	2.5	2.0	1.0	1.0	1.0	0.5	0.5	2.0	4.5	4.0	2.5	4.5	2.0	1.0	0.
65000,5.30,0.09	3.0	3.5	4.5	4.0	4.0	3.0	2.0	1.0	1.5	1.0	0.5	0.	2.0	5.0	4.0	0.	5.0	4.0	1.0	0.
51000,4.50,0.09	1.5	2.5	5.0	4.0	6.0	4.0	2.0	0.5	3.0	2.0	1.0	0.5	1.0	4.0	2.5	1.0	6.0	1.5	0.5	0.
38000,4.25,0.09	2.5	3.5	4.5	3.5	4.0	2.0	1.0	0.	1.5	1.0	0.5	0.	2.0	3.5	2.0	1.0	5.0	1.0	0.	0.
33000,4.15,0.09	1.0	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0	2.0	1.0	0.5	1.0	0.5	0.	0.
75000,5.00,0.99	5.0	5.5	6.5	5.0	6.5	5.0	2.5	1.0	3.0	2.0	1.0	0.5	2.5	4.5	3.5	2.0	6.5	2.0	1.0	0.
65000,5.00,0.99	4.0	5.0	6.0	4.5	7.0	4.5	2.0	1.0	3.5	2.0	1.0	0.5	2.5	4.5	3.5	2.0	6.5	2.0	1.0	0.
50000,5.00,0.99	3.5	5.0	6.0	4.0	6.5	4.0	2.0	1.0	3.0	2.0	1.0	0.	2.0	4.5	3.5	2.0	7.0	2.0	0.5	0.
40000,4.00,0.99	2.5	3.5	5.5	3.5	8.0	4.0	1.5	0.5	5.5	2.0	1.0	0.	1.5	3.0	2.5	1.0	4.5	1.5	0.5	0.

Table 3.8 – Total percentage changes in the residual intensity of several Helium lines for different models. $\Delta\lambda$ are given in Å. New profiles are deeper. The models are identified by T_{eff} , $\log g$ and Y .

III.3.4. – Comparison with the Observations

As for Hydrogen, we obtain new theoretical profiles for Helium that are deeper than the *standard* ones. Although the effects are smaller than for Hydrogen we wish to show here that they can affect the results of the spectroscopic analysis, especially in the case of very high quality observations.

We will use the $\lambda 4686$ line. This line is the most relevant in the visible spectrum of HeII, although it sometimes cannot be considered for the analysis due to the breakdown of the physical assumptions we have employed (see the discussion concerning Of stars in the Introduction).

We start again with τ Sco. The adopted parameters and references are the same as for Hydrogen. Fig. 3.21 shows both theoretical profiles, including convolution with an instrumental profile with a FWHM = 0.35 Å and a rotational profile of 5 km/s. This is made to ensure that the small effect shown by our calculations at these stellar parameters not disappear due to these smoothing functions. It can be seen in the figure that the core is too deep in both cases, but in our calculations the wings are also stronger than observed. This is not clearly seen in the *standard* calculations. Thus our new profiles point to temperatures and/or Helium abundances slightly lower than adopted by Schönberner *et al.* (1986). The Balmer line profiles could then be slightly deeper as well, but this does not affect the conclusions presented in the Hydrogen discussion.

Our second example is the O9V star 10 Lac, also recently studied by Schönberner *et al.*. These authors assigned a T_{eff} of 38000 K, a $\log g$ of 4.25 and a normal abundance of Helium, $Y = 0.09$ to it. The adopted rotational velocity is 25 km/s, and the instrumental profile has a FWHM of 0.35 Å.

We show the profiles in Fig. 3.22. Although the changes are now greater than for τ Sco, this is compensated by the fact that the observed data are of poorer quality so that there is no indication that corrections to the stellar parameters are needed, especially considering the better fit of the core by our calculations.

Our more interesting case is again the CPN NGC 1360. Méndez *et al.* (1985) assigned to this object a Helium abundance of $Y = 0.05$, with $T_{\text{eff}} = 60000$ K and $\log g = 5.2$. As we have seen for Hydrogen, the temperature of this star is somewhat hotter; we adopted there $T_{\text{eff}} = 75000$ K, $\log g = 5.5$. But the equivalent width of $\lambda 4541$ would be too small compared with the observations if the Helium abundance is kept at the value proposed by Méndez *et al.*, as in this temperature region the equivalent width of this line decreases when the temperature increases. On the other hand, the equivalent width of HeII $\lambda 4686$ increases with the temperature. However, for this line we use new unpublished observational data kindly provided by Dr. Méndez. These data have again been obtained using the CASPEC spectrograph plus CCD attached to the ESO 3.6 m telescope. The new observational profile is deeper than the one used by Méndez *et al.* so that our new calculations at a hotter temperature and *normal Helium abundance* are able to fit it surprisingly well, as is shown in Fig. 3.23. The *standard* calculations at 60000 K

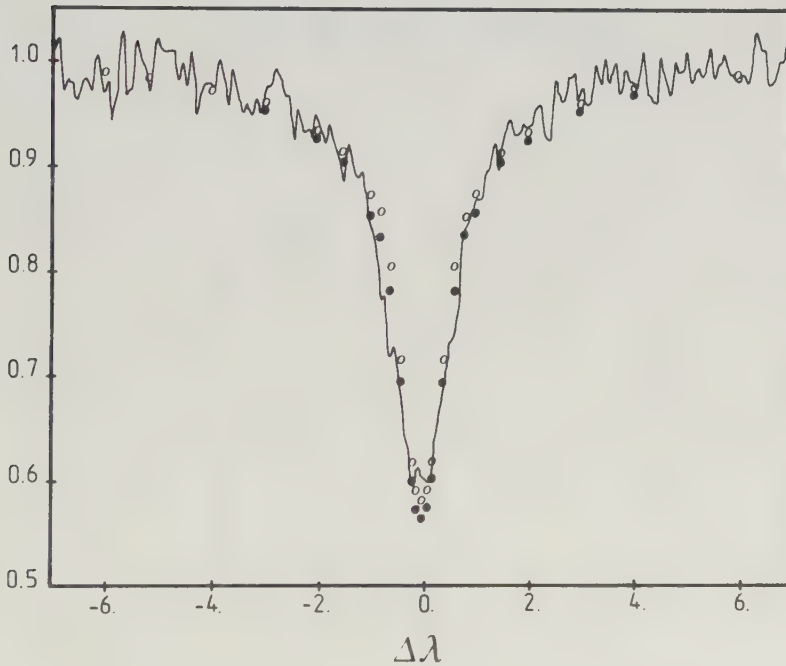
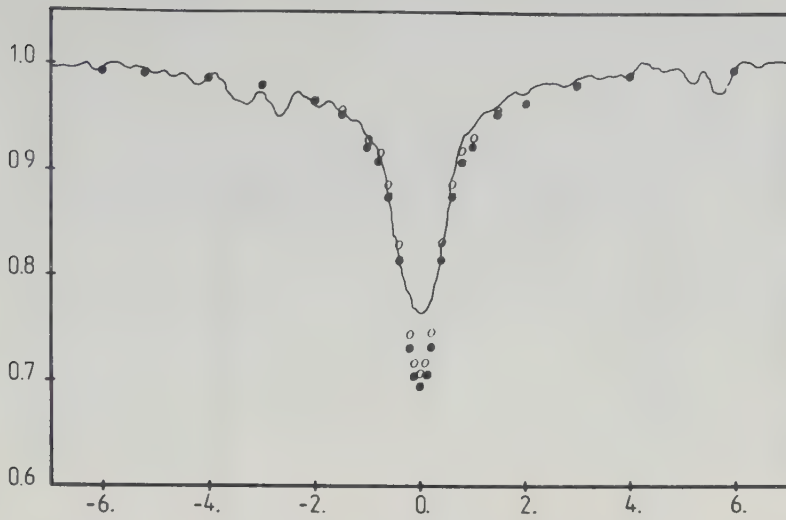


Fig. 3.21 : The $\lambda 4686$ profile of τ Sco. Open circles: *standard* calculations with $T_{\text{eff}} = 33000$, $\log g = 4.15$, $Y = 0.10$ and $v \sin i = 5$ km/s. Filled circles: our calculations for the same parameters.

Fig. 3.22 : Same as Fig. 3.21 for 10 Lac, with $T_{\text{eff}} = 38000$, $\log g = 4.25$, $Y = 0.09$ and $v \sin i = 25$ km/s.

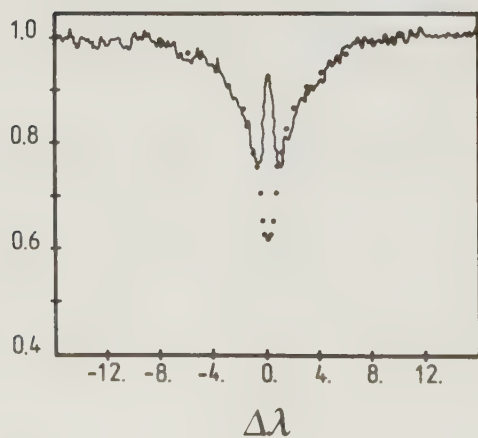
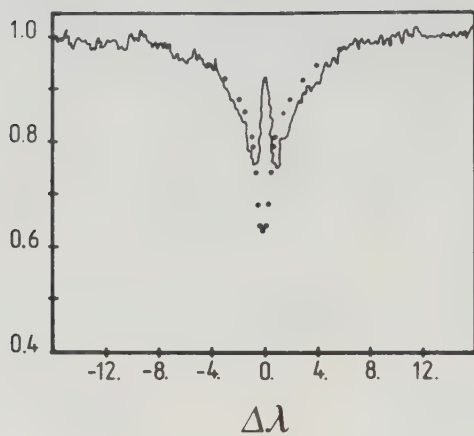


Fig. 3.23a and 3.23b: The $\lambda 4686$ profile of NGC 1360 with $T_{\text{eff}} = 75000$, $\log g = 5.5$ and $Y = 0.09$. Upper: *standard* calculations; lower: our calculations.

and $Y = 0.05$ cannot fit the observational profile, as both parameters will strongly reduce the equivalent width of the line. Also the *standard* calculations with the new stellar parameters produce line wings that are too shallow.

Thus we conclude that NGC 1360 is an object hotter than previously assumed (an effect found by the use of the new calculations) and with nearly normal Helium abundance (nearly a factor of two more than the former analysis, an effect due to the combination of improved theoretical profiles with better observational data). The conclusion that the spectroscopic analysis of *Méndez et al* (1985) must be revised is thus reinforced, as not only the temperatures but also the Helium abundances are influenced by the effects described here.

III.4. – The Overlapping of Hydrogen and Ionized Helium

As a last problem we treat the overlapping between the Hydrogen lines and the corresponding Helium lines. As we have seen in the Introduction, this overlapping could contribute to the $\lambda 4686$ emission in Of stars by pumping the electrons from level 2 to level 4 of HeII with photons of the L_{γ} - α line of HI (Bowen mechanism), although sphericity is probably the major cause (*Kunasz et al.*, 1975). *Auer and Mihalas* (1972) could not reach any clear conclusion with their two extreme assumptions of exact coincidence and no overlap. *Mihalas and Lockwood* (1972) showed that the calculations without overlap are in closer agreement with the observations than those considering exact coincidence of the HI and HeII lines. These were, however, rough qualitative estimates; we wish to quantify here the actual importance of the full overlap in stellar photospheres. Thus it is not possible in this case to compare with previous calculations.

We use the same Hydrogen atom as described in II.2., i.e., a model with 10 NLTE levels and Stark broadening for all transitions whose upper level is $n_{up} \leq 7$. For Helium we use a similar 10 NLTE level atom with Stark broadening for the same lines as for Hydrogen. Neglect of the upper levels is here unimportant, inasmuch as we study the effect of the overlapping differentially.

We start by performing the line formation calculations for Hydrogen and Helium separately. Then, Hydrogen is again iterated to see if the new populations of Helium influence the H populations. Finally the whole overlap is treated. In this

case we have a total of 111 transitions (90 bound – bound and 21 bound – free). To limit the number of frequency points and save computing time only one frequency grid is used when two lines overlap in their wings. The cores of the lines, however, are always explicitly included in the frequency grid (by *core* we mean here all frequencies such that $|\nu - \nu_c| \leq 2\Delta\nu_D$). Our final grid has 1100 frequency points.

The γ 's used were those employed in the Helium calculations. In addition the ground state continuum of HeII was treated as in those calculations, as were the resonance lines. All other continua were treated with the Λ iteration. The convergence required was 10^{-3} .

III.4.1. – Numerical Results

We have chosen a model with $T_{\text{eff}} = 42000$, $\log g = 3.5$ and $Y = 0.14$ to study the problem. These parameters represent the final fit of *Kudritzki et al.* (1983) to ζ Puppis. As already stated in the Introduction, this is an extreme Of star, so that the $\lambda 4686$ line of HeII appears in emission, contrary to the predictions of plane – parallel models. We may then expect the effect of the overlapping to be stronger in this star than in others, whose spectra can be explained by our Helium line formation calculations.

The initial separated line formation calculations of Hydrogen and Helium give the same results as described in the preceding sections. When we iterate the occupation numbers of Hydrogen again after the Helium line formation, only the ground level population changes very slightly, namely of the order of 1%. These changes do not affect the calculated profiles that remain the same as before. They are also too small to alter the Helium populations.

The changes in the occupation numbers of several levels of HeII after the line formation calculations including overlap are schematically shown in Fig. 3.24. The changes in the occupation numbers of Hydrogen are again very small and do not need to be considered.

To understand the mechanism that changes the occupation numbers of HeII we take level $n = 4$ as an example (to investigate the possible action of the

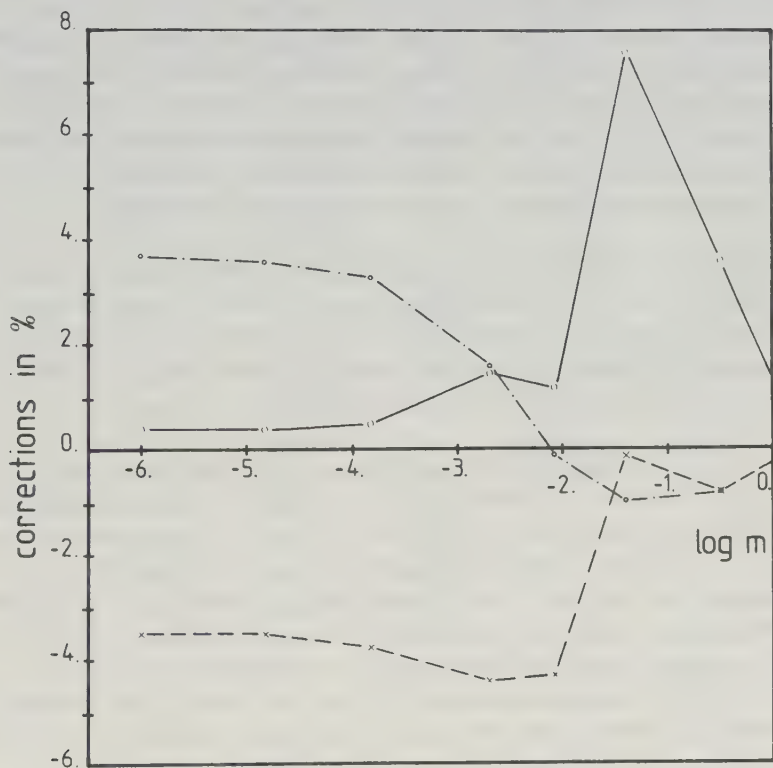


Fig. 3.24: Percentage changes in the occupation numbers of several HeII levels after inclusion of the overlap with HI. Full drawn: $n=2$; (— —): $n=4$; (— · —): $n=10$. The ground level behaves like $n=2$; levels 3, 5 and 6 behave like $n=4$; levels 7, 8 and 9 behave like $n=10$. The model has $T_{\text{eff}}=42000$, $\log g=3.5$ and $Y=0.14$. Again, only some representative depth points are shown.

Bowen mechanism). Table 3.9 contains the net radiative rates per atom in level $n = 4$ of transitions involving this level. Case a) displays the rates without overlapping with Hydrogen and case b) includes overlapping, but *before we iterate the occupation numbers of Helium*. This will indicate in which direction (population or depopulation of the level) the previous equilibrium is displaced due to the new radiation field and opacities. It should be noted that argumentation using the *final* net radiative rates is actually not useful as then the collisional rates will also change and, worse, the net rates (both radiative and collisional) *include the changes in the occupation numbers already*, so that the argument would be circular.

The numbers in Table 3.9 should be interpreted as follows: negative numbers indicate that the downward rates dominate, positive numbers indicate domination of the upward rates. The difference between cases a) and b) gives the trend in each transition. Transitions that do not overlap with Hydrogen lines will not change. (Line $4 \leftrightarrow 5$ of HeII overlaps with the $3 \leftrightarrow 7$ transition of HI).

We can see from Table 3.9 that the tendency in the outer layers is to depopulate level $n = 4$ (upward rates increase). Moreover, the upper levels and the level $n = 2$ are repopulated. (Although $n = 2$ is depopulated compared with $n = 4$ in the deeper layers, a consequence of the local emission of $L_{\gamma} - \alpha$ in comparison with the local Planck function, as was pointed out by *Auer and Mihalas* (1972)). This interpretation seems to be wrong for $\log m = -0.5$: level 4 is depopulated although the tendency points to a repopulation. The explanation is simply that so deep in the atmosphere the effect of the collisions is very strong and maintains the coupling between all levels. Thus the $n = 4$ level does not control its own changes; instead all upper levels ($n \geq 3$) change together.

We wish to point out that the Bowen mechanism is actually in operation: the number of electrons cascading from level 4 to level 3 increases as a consequence of the overlap, although only at the 2% level. However, because of the fact that $n = 3$ is in total less depopulated than $n = 4$ the emergent flux decreases (very slightly).

Although the percentage changes in the occupation numbers of HeII are relatively large, the corresponding changes in the profiles are small: in the centre of the lines $\lambda\lambda$ 5411 ($4 \leftrightarrow 7$), 4686 ($3 \leftrightarrow 4$) and 4541 ($4 \leftrightarrow 9$) they are respectively +2.5%, -1.4% and -0.5%. The changes away from the centre become rapidly smaller.

		log m					
transition		0.55	-0.50	-1.38	-2.10	-2.85	-3.80
2 $\leftrightarrow$ 4	Case a	6.0417 10 ⁴	1.6873 10 ⁵	3.4043 10 ⁶	7.9232 10 ⁶	-1.2753 10 ⁷	-1.6279 10 ⁷
	Case b	2.1929 10 ⁴	1.4791 10 ⁵	3.3379 10 ⁶	8.2895 10 ⁶	-1.2091 10 ⁷	-1.5605 10 ⁷
	trend	-3.849 10 ⁴	-2.0811 10 ⁴	3.3379 10 ⁶	8.2895 10 ⁶	6.62 10 ⁵	6.74 10 ⁵
3 $\leftrightarrow$ 4	a	-1.3967 10 ⁴	1.4476 10 ⁵	6.0160 10 ⁵	3.1078 10 ⁷	8.6673 10 ⁷	9.2259 10 ⁷
	b	-1.4066 10 ⁴	1.4463 10 ⁵	6.0159 10 ⁵	3.1078 10 ⁷	8.6673 10 ⁷	9.2259 10 ⁷
	trend	-9.90 10 ²	-1.30 10 ²	-1.00 10 ¹	0.	0.	0.
5 $\leftrightarrow$ 4	a	1.9734 10 ⁴	-3.6860 10 ⁴	-2.0315 10 ⁵	-1.1319 10 ⁷	-2.7753 10 ⁷	-2.8333 10 ⁷
	b	1.5501 10 ⁴	-7.2200 10 ³	-3.1841 10 ⁶	-1.1357 10 ⁷	-2.7771 10 ⁷	-2.8944 10 ⁷
	trend	-4.233 10 ³	2.694 10 ⁴	-1.1526 10 ⁵	-3.80 10 ⁴	-1.80 10 ⁴	-1.10 10 ⁴
6 $\leftrightarrow$ 4	a	1.2548 10 ⁴	-7.1760 10 ⁴	-4.4278 10 ⁵	-7.3109 10 ⁶	-1.1640 10 ⁷	-1.1473 10 ⁷
	b	-7.1818 10 ⁴	-1.0963 10 ⁵	-4.5409 10 ⁵	-7.3143 10 ⁶	-1.1641 10 ⁷	-1.1473 10 ⁷
	trend	-8.4366 10 ⁴	-3.787 10 ⁴	-1.131 10 ⁴	-3.40 10 ³	-1.00 10 ³	0.
7 $\leftrightarrow$ 4	a	8.6482 10 ³	-8.5300 10 ⁴	-6.7537 10 ⁵	-3.6979 10 ⁶	-5.4092 10 ⁶	-5.2038 10 ⁶
	b	8.7072 10 ³	-8.5120 10 ⁴	-6.7530 10 ⁵	-3.6979 10 ⁶	-5.4092 10 ⁶	-5.2038 10 ⁶
	trend	5.90 10 ¹	1.80 10 ²	7.00 10 ¹	0.	0.	0.
8 $\leftrightarrow$ 4	a	1.4296 10 ³	-3.6412 10 ³	-7.5861 10 ⁵	-2.2507 10 ⁶	-3.2019 10 ⁶	-2.9312 10 ⁶
	b	-4.5728 10 ³	-9.3217 10 ³	-6.9955 10 ⁵	-2.0933 10 ⁶	2.9763 10 ⁶	2.7241 10 ⁶
	trend	-6.0024 10 ³	-5.6805 10 ³	5.9060 10 ⁴	1.5740 10 ⁵	2.256 10 ⁵	2.071 10 ⁵
9 $\leftrightarrow$ 4	a	1.2888 10 ³	-1.7365 10 ⁴	-5.5283 10 ⁵	-1.5370 10 ⁶	-2.2395 10 ⁶	-2.0049 10 ⁶
	b	1.2958 10 ³	-1.7325 10 ⁴	-5.5279 10 ⁵	-1.5368 10 ⁶	-2.2394 10 ⁶	-2.0048 10 ⁶
	trend	7.00 10 ⁰	4.00 10 ¹	4.00 10 ¹	2.00 10 ¹	1.00 10 ²	1.00 10 ²
10 $\leftrightarrow$ 4	a	1.1790 10 ²	-3.3301 10 ⁴	-3.9856 10 ⁵	-1.0814 10 ⁶	-1.6343 10 ⁶	-1.4196 10 ⁶
	b	-3.0409 10 ³	-3.2604 10 ⁴	-3.7236 10 ⁵	-1.0075 10 ⁶	1.5204 10 ⁶	1.3208 10 ⁶
	trend	-4.0588 10 ³	6.97 10 ²	2.62 10 ⁴	7.39 10 ⁴	1.139 10 ⁵	9.88 10 ⁴
k $\leftrightarrow$ 4	a	-2.0690 10 ⁶	-4.2811 10 ⁶	-2.9041 10 ⁶	-1.1815 10 ⁷	-2.1983 10 ⁷	-2.4602 10 ⁷
	b	-2.0480 10 ⁶	-4.2749 10 ⁶	-2.9037 10 ⁶	-1.1825 10 ⁷	-2.1999 10 ⁷	-2.4621 10 ⁷
	trend	2.10 10 ⁴	6.20 10 ³	4.00 10 ²	-1.00 10 ⁴	-1.60 10 ⁴	-1.90 10 ⁴
Total	a	-1.9788 10 ⁶	-4.2158 10 ⁶	-1.9295 10 ⁶	-1.070 10 ⁴	+5.91 10 ⁴	+1.25 10 ⁴
	b	-2.0950 10 ⁶	-4.2436 10 ⁶	-2.0367 10 ⁶	+5.3570 10 ⁵	+1.0257 10 ⁶	+9.625 10 ⁵
	trend	-1.1618 10 ⁵	-2.78 10 ⁴	-1.0721 10 ⁵	+5.464 10 ⁵	+9.666 10 ⁵	+9.50 10 ⁵

Table 3.9 - The net radiative rates per atom in level $n = 4$ of the transitions involving this level.

Case a: no overlapping; case b: overlapping, before the iteration process. Trend: difference between b and a. Positive numbers indicate that electrons leave level $n = 4$.

To explain why the profiles do not vary, we repeat formula (3.1). This gives, for some frequency, the flux at the surface:

$$H_{\nu}(0) = 1/4 S_{\nu}(\tau_{\nu} = 2/3) \quad (3.1)$$

The source function for transition $i \rightarrow j$ is

$$S_{ij} = (2h\nu^3/c^2) [(n_i g_j / n_j g_i) - 1]^{-1} = (2h\nu^3/c^2) [(b_i/b_j)(n_i^* g_j / n_j^* g_i) - 1]^{-1} \quad (3.8)$$

where b_i, b_j are the departure coefficients. From the Boltzmann formula

$$n_i^* / n_j^* = (g_i / g_j) e^{(\chi_i - \chi_j) / kT} = (g_i / g_j) \alpha(T) \quad (3.9)$$

χ_i and χ_j being the ionization energies of the levels with respect to the continuum. We may then write

$$S_{ij} = (2h\nu^3/c^2) [(\alpha(T) b_i/b_j) - 1]^{-1} \quad (3.10)$$

Thus the source function - and consequently the emergent profile - will change only when the ratio b_i/b_j at the formation depth changes and not when the departure coefficients or the occupation numbers themselves change.

Table 3.10 shows the ratios b_4/b_7 , b_3/b_4 and b_4/b_9 throughout the atmosphere, before and after consideration of the overlap.

	log m	- 6.50	- 4.80	- 3.80	- 2.85	- 2.10	- 1.38	- 0.50	+ 0.55
Ratio									
b_4/b_7		0.994	0.993	0.979	0.951	1.140	1.329	1.093	1.010
		0.865	0.864	0.853	0.834	1.051	1.335	1.094	1.010
b_3/b_4		1.154	1.153	1.148	1.200	1.491	1.162	1.031	1.018
		1.153	1.152	1.147	1.201	1.504	1.163	1.032	1.017
b_4/b_9		0.969	0.965	0.937	0.869	1.072	1.344	1.100	1.010
		0.768	0.767	0.758	0.750	1.002	1.359	1.102	1.010

Table 3.10 - Ratio of several departure coefficients, before (upper numbers) and after (lower numbers) consideration of the overlapping.

We cannot expect great changes in the emergent flux of the $3\leftrightarrow 4$ transition after examination of Table 3.10. For transitions $4\leftrightarrow 7$ and $4\leftrightarrow 9$, however, variations are possible. The formation depths of the lines are $\log m \approx -1.38$, -1.95 and -1.00 for $4\leftrightarrow 7$, $3\leftrightarrow 4$ and $4\leftrightarrow 9$ respectively. At the corresponding depths the ratios have changed only very slightly, which explains why the emergent profiles are the same as before.

If we look at Fig. 3.24 and use the above arguments, we conclude that the emergent profiles of the lines connecting level $n = 2$ with the upper levels must change. Inspection of the $2\leftrightarrow 3$ line at $\lambda 1640$ shows that the residual intensity changes by 4.0% at $\Delta\lambda = 0\text{\AA}$, 1.0% at $\Delta\lambda = 0.4$ and 0.1% at $\Delta\lambda = 1$. The UV lines of the $n = 2$ series of HeII are thus affected by the overlap with HI. This conclusion is not affected by the assumption of detailed balancing in the resonance lines, as these are formed higher in the atmosphere than those from $n = 2$, especially the $1\leftrightarrow 2$ line. Unfortunately, the $n = 2$ lines are very difficult to use for quantitative spectroscopy, both because they lie in the UV and because they are usually formed in the uppermost layers of the star.

Results for other model atmospheres have been analyzed, looking for more important effects of the overlapping phenomena. We have calculated models with $Y = 0.5$ (where the increased Helium content could perhaps favour the interaction between both atoms), and models with higher temperatures (where the Hydrogen lines, becoming more transparent, could "illuminate" the Helium ones). The results, listed in Table 3.11, are qualitatively similar to those of ζ Puppis and quantitatively of the same order. Even the reiteration of Hydrogen after the Helium line formation produces changes in the Hydrogen populations only of the order of 1% in models with $Y = 0.5$, and do not alter the profiles.

Thus we must conclude that the overlapping of Hydrogen and Helium lines is of no importance for the optical lines in stellar photospheres. In particular, the Bowen mechanism is not effective in the analyzed models and cannot explain, even partially, the $\lambda 4686$ emission. Only a small effect is present in the UV lines belonging to level $n = 2$.

We conclude that Hydrogen and Helium line formation calculations can be performed separately.

Model	Line	4↔7			4↔9			3↔4		
	$\Delta\lambda =$	0	0.4	2	0	0.4	2	0	0.4	2
75000,5.5,0.09	0.5	0.5	0.		0.	0.	0.	0.	1.0	1.0
51000,4.5,0.09	0.5	0.	0.		1.0	1.0	0.	1.0	1.0	0.5
50000,4.0,0.09	-1.5	0.	0.		0.	0.5	0.	0.	0.5	0.
42000,3.5,0.14	-2.5	0.5	0.		0.5	0.5	0.	1.5	0.5	0.
75000,5.0,0.50	0.5	1.0	0.5		0.5	0.5	0.	0.5	0.5	1.0
50000,3.8,0.50	-2.0	0.	0.		0.5	0.5	0.	1.5	0.5	0.
35000,3.5,0.50	2.0	1.0	0.		0.5	0.	0.	-1.0	0.	0.5

Table 3.11 - Total percentage changes in the residual intensities of some lines of HeII after inclusion of the H-HeII overlapping. Negative numbers indicate that the new profiles are shallower. The $\Delta\lambda$ are given in Å and the models are identified by T_{eff} , $\log g$ and Y .

CHAPTER IV

Summary and Conclusions

In the work presented here we have applied the new technique of the Accelerated Lambda Iteration (*Werner and Husfeld, 1985*) to multilevel line formation problems of Hydrogen and Helium II. The model atmospheres used cover a wide range of temperatures and gravities (from 30000 K to 75000 K in T_{eff} , and from 3.5 to 6.5 in $\log g$). In addition, three different Helium abundances were used corresponding to normal, intermediate, and extreme Helium rich objects. These models are appropriate for O, sdO and sdOB stars and for some Central stars of Planetary Nebulae.

The technique and our program based on it have been tested by comparing with previous calculations. In all cases excellent agreement was achieved.

In a first step we performed new and more detailed Hydrogen line formation calculations by including more levels and Stark broadening calculations in the statistical equilibrium equations and analyzed the effects of these improvements on the occupation numbers and emergent profiles. It was shown that the additional upper levels act as channels through which electrons cascade to the lower ones when the corresponding lines become optically thin. The inclusion of Stark broadening produces changes in deep layers when, due to the complete redistribution approximation, photons, earlier trapped in the core, escape through the far wings; and in middle layers due to the additional opacity in the near wings. At the same time, it was shown that the depth-dependence of the Doppler profiles has no importance.

The changes in the occupation numbers induce changes in the emergent profiles. The direction of these changes (if the new profiles are deeper or shallower) depends on the relative changes of the corresponding upper and lower levels. It was shown that for H_{β} and H_{γ} the new profiles are deeper. To achieve sufficient accuracy for comparison with the new high quality observations we conclude that the Hydrogen atom must be described by a model including 10 NLTE levels and all transitions coupling them. Stark broadening must be consi-

dered in the statistical equilibrium equations for all lines with $n_{\text{upper}} \leq 7$. This represents a total of 55 transitions and 600 frequency points (a factor 10 greater than the *standard* calculations).

The above described effects are present for all models. They produce H_{β} and H_{γ} profiles with residual intensities that are approximately 10% deeper in the line centre, 4% at $\Delta\lambda = 1 \text{ \AA}$ and 1.5% at $\Delta\lambda = 2 \text{ \AA}$. The additional levels have a contribution to these values somewhat greater than the Stark broadening.

When we compare with the observations, the new profiles, being deeper, resolve the discrepancy between observed and *standard* calculated cores of Balmer profiles in slow rotators. Because the effects are present in all models, we conclude that they are masked by rotation in other stars. Our new calculations are specially important for the quantitative spectroscopy of CPN, where the ionization balance of Helium cannot be used for the determination of T_{eff} and instead the core of the Balmer lines must be employed.

In a second step we performed HeII calculations similar to those for Hydrogen. However, for HeII some approximations were made concerning the resonance lines and the ground level continuum. These transitions were set in detailed balancing when they became extremely thick. The former were kept in detailed balancing for all models, the latter for models with $T_{\text{eff}} \leq 50000 \text{ K}$ (if they were extreme or intermediate Helium models) or $T_{\text{eff}} \leq 38000 \text{ K}$ (if they had normal Helium abundance). We tested these approximations by relaxing them for some models. No changes appeared in the calculated emergent profiles.

The variations of the occupation numbers and emergent profiles after introduction of more levels and Stark broadening in the statistical equilibrium equations are qualitatively the same as for Hydrogen. Quantitatively they are smaller because the number of levels included in the *standard* calculations was appropriate. We conclude that the Helium II atom must be described by a 14 NLTE level atom model including all transitions coupling them. As for Hydrogen, Stark broadening must be considered for lines with $n_{\text{upper}} \geq 7$. We have then a total of 93 transitions and 650 frequency points (again a factor of 10 greater than the *standard* calculations).

When comparing with the observations the new profiles also give better fits.

Lastly we have calculated for the first time the full overlap of Hydrogen and Helium II lines. The Hydrogen atom was treated as in the Hydrogen calculations, the Helium II atom was simplified to a 10 NLTE level atom. Stark broadening was included for the same lines as before. The total number of NLTE levels was 23, coupled by 102 transitions described by 1100 frequency points.

In the calculations previous to the full overlap it was found that Hydrogen does not need to be recalculated after solution of the Helium line formation, even for intermediate Helium rich models.

Our computations show that the occupation numbers of Hydrogen do not change as a consequence of the overlap. On the other hand, the occupation numbers of Helium II are changed, but the optical profiles are not, as the ratio of the departure coefficients remain unaltered in the corresponding line formation layers. An effect can be seen in the core of the UV lines belonging to the series of level $n = 2$ but these lines are often formed in the uppermost layers of the atmosphere and are not very useful for quantitative spectroscopy.

Thus the overlap has no influence on the optical profiles of H and HeII. In particular only very small changes are found for $\lambda 4686$. We conclude that the Hydrogen and Helium line formation calculations can be separately performed, as had been done previously.

We wish to say here a few words about possible work in the future. Evidently, the technique may be extended to other ions. For the stars treated here HeI and the ions belonging to the CNO elements (CIII, CIV, NIII, NIV, NV, OII, OIII) are the most important. The first is needed for an exact determination of the HeI/HeII ionization balance and for the analysis of stars cooler than 30000 K. The second should give us the abundances of the corresponding elements which are closely related to the evolution of those stars and are essential for the study of objects such as the OBN stars.

Another application is the construction of NLTE model atmospheres including line blanketing. This mechanism can change the whole temperature structure and the background opacities in the atmospheres. Work is currently under way to

investigate this important point (*Werner, 1986; Kunze, 1986*).

The technique can be extended to all problems needing a great number of frequency (or angle - frequency) points, like those of including partial redistribution functions (which have never been considered in multilevel line formation calculations) or velocity fields. The last subject have already been treated by *Hamann* (1985), who applied the technique to expanding envelopes with spherical geometry, which, as we have seen, probably plays an important role in a great number of stars. Spherical models are badly needed and their calculation is presently under way (*Gabler, 1986; Wagner, 1986*) with standard techniques.

Finally our results show the importance of the calculation of a new grid of H/He line formation models, especially for CPN where the effects are greater and the stars need to be placed in the HR diagram with higher accuracy than has been hitherto possible. Of course, such a grid would be applicable not only to CPN, but also to O, sdO and sdOB stars. This work is already in progress.

APPENDIX

Atomic Data and Formulae

In this appendix we wish to present the data and formulae used in the calculation of the opacities, emissivities and rates described in Chapter II. The necessary energies are taken from the Atomic Energy Levels of *Moore* (1949).

A.1. - Free - Free Opacities

The free - free absorption coefficient of Hydrogen per proton and electron may be written (*Mihalas*, 1978, pg.101)

$$\alpha_{\nu} = (4e^6 Z^2 / 3ch) (2\pi / 3km^3)^{1/2} T^{-1/2} \nu^{-3} \bar{g}_{III}(\nu, T) \quad (A.1)$$

The free - free Gaunt factors are given by *Mihalas* (1967), who fitted the values obtained by *Berger* (1956) to an analytical formula:

for $\lambda > 10^4 \text{ \AA}$

$$\bar{g}_{III}(\nu, T) = (1.0823 + 2.98 \times 10^{-2} / \theta) + (6.7 \times 10^{-3} + 1.12 \times 10^{-2} / \theta) \lambda_{\mu} \quad (A.2)$$

for $10^2 < \lambda < 10^4 \text{ \AA}$

$$\bar{g}_{III} = C_1 + C_2 \lambda_{\mu} + C_3 \lambda_{\mu}^2 + C_4 \lambda_{\mu}^3 \quad (A.3)$$

$$\text{with } C_i = C_{i1} + C_{i2} / \theta + C_{i3} / \theta^2 \quad (A.4)$$

where λ_{μ} is the wavelength in microns and

$$\theta = 5040 / T \quad (A.5)$$

The coefficients are given in Table A.1

	C_{i1}	C_{i2}	C_{i3}
C_1	1.070192	3.9999187×10^{-3}	$-7.8622889 \times 10^{-5}$
C_2	0.26061249	6.4628601×10^{-2}	$-6.1953813 \times 10^{-4}$
C_3	-0.57917786	$-3.7542343 \times 10^{-2}$	$-1.3983474 \times 10^{-5}$
C_4	0.34169006	1.1852264×10^{-2}	0.

Table A.1 – Fit coefficients for the formula (A.4)

Mihalas tested the formula between 5800 and 120000 K, where the agreement with Berger's values is better than 1%.

These formulae may also be used for ionized He. Only a few small differences must be kept in mind: i) the absorption coefficient is given per alpha particle and not per proton, ii) now $Z = 2$, iii) the frequencies must be scaled by $1/Z^2$ for the Gaunt factor calculation.

The HeI free-free opacity will be calculated with the formulae (A.1)–(A.5) too. Our treatment of the HeI atom, considering it as hydrogenic for states $n \geq 2$ has been justified in Chapter III.

The last source of opacity we consider is that of electron scattering. The absorption coefficient per electron is a constant,

$$\sigma_e = (8\pi e^4 / 3m^2 c^4) = 6.650 \times 10^{-25} \text{ cm}^2 \quad (\text{A.6})$$

The numerical values are taken from *Allen* (1973)

A.2. – Bound – Free Opacities

The bound – free absorption coefficient per absorbing atom in level n may be written for H

$$\alpha_{\nu} = (64\pi^4 m e^{10} / 3\sqrt{3} h^6) 1/(n^5 \nu^3) \bar{g}_{II}(n, \nu) \quad (\text{A.7})$$

where $\bar{g}_{II}(n, \nu)$ is the bound – free Gaunt factor for level n at frequency ν . We have adopted the values of Gingerich (1964), who approximated g_{II} with the form

$$\bar{g}_{II}(n, \nu) = a_n + b_n \nu^{-1} + c_n \nu^{-2} \quad (\text{A.8})$$

The coefficients for the three lower states of Hydrogen are given in Table A.2. For $n > 3$, $\bar{g}_{II}(n, \nu)$ has been set equal to 1.

n	a_n	b_n	c_n
1	0.9916	2.71852×10^{13}	-2.26846×10^{30}
2	1.105	-2.37496×10^{14}	4.07677×10^{28}
3	1.101	-9.863186×10^{13}	1.03537×10^{28}

Table A.2 – Coefficients for the bound – free Gaunt factors in formula (A.8)

For levels with principal quantum number $n' \geq n$ (n being the lowest level not explicitly considered in the calculations) an estimate of their contribution to the opacity at frequency ν may be obtained by integrating (A.7) over all appropriate levels (i.e., we suppose $\Delta n = 1 < n$) (Unsöld, 1968, pg.169). By writing the coefficient per electron and proton (with the use of Saha – Boltzmann formula), we obtain

$$\alpha_{\nu} = (4e^6 Z^2 / 3ch) (2\pi / 3km)^{1/2} T^{-1/2} \nu^{-3} (e^{-u_n} - 1) \quad (\text{A.9})$$

where $u_n = \chi_n / kT$, χ_n being the energy of level n with respect to continuum.

Comparison of (A.9) and (A.1) indicate that the contribution of the upper levels may be treated in the same manner as the free – free opacity.

The HeII bound - free absorption coefficients are calculated with the formulae (A.7) and (A.9) as well. Only the coefficients in (A.8) need to be scaled: b_n should be multiplied by 4 (Z^2), c_n by 16 (Z^4). (A.9) must be interpreted as being per alpha particle.

In addition, the upper levels of HeI ($n \geq 2$) are treated with the same formulae. (A.9) is to be interpreted as that for a HeII atom in the ground level.

Finally, for the ground level of HeI the expression of *Hunger and Van Blerkom* (1967) is used:

$$a_v = 2.951209 \times 10^{14} v^{-2} \quad (\text{A.10})$$

A.3. - Bound - Bound Opacities

In the stellar photospheres of hot stars, the line profiles of Hydrogen and Helium are broadened by two dominating mechanisms: Doppler broadening (due to the high temperatures) and Stark broadening (due to the high densities).

The Doppler broadened absorption coefficient at frequency v per absorbing atom (i.e., per atom in the lower level), may be written:

$$\sigma_{ij}(v) = (\pi^{1/2} e^2 / mc) f_{ij} 1/\Delta v_D e^{-(\Delta v / \Delta v_D)^2} \quad (\text{A.11})$$

where i and j are the lower and upper levels of the transition, Δv is the frequency distance from the line center and Δv_D is the Doppler width

$$\Delta v_D = v_c / c (2kT/m)^{1/2} \quad (\text{A.12})$$

v_c being the central frequency of the line. The quantity f_{ij} is the oscillator strength, obtained from quantum - mechanical calculations or experiment. For our Hydrogen and Helium lines we use the formula of *Johnson* (1972)

$$f_{ij} = (32/3\sqrt{3} \pi) (n_i/n_j^3) X^{-3} g(i,X) \quad (\text{A.13})$$

Here, n_i and n_j are the principal quantum numbers of levels i and j and X is the ratio of the transition energy to the ionization energy of the lower level

$$X = E_{ij}/I_i = 1 - (n_i/n_j)^2 \quad (\text{A.14})$$

and $g(i,X)$ is a correction factor that is continuous with the Gaunt factor for bound - free transitions as $n_j \rightarrow \infty$. It may be approximated by

$$g(i,X) = g_0(i) + g_1(i) X^{-1} + g_2(i) X^{-2} \quad (\text{A.15})$$

The coefficients are given in Table A.3

	$n = 1$	$n = 2$	$n \geq 3$
g_0	1.1330	1.0785	$0.9935 + 0.2328 n^{-1} - 0.1296 n^{-2}$
g_1	-0.4059	-0.2319	$-n^{-1} (0.6282 - 0.5598 n^{-1} + 0.5299 n^{-2})$
g_2	0.07014	0.02947	$n^{-2} (0.3887 - 1.181 n^{-1} + 1.470 n^{-2})$

Table A.3 - Coefficients for (A.15)

The formula of Johnson reproduces the oscillator strengths calculated by *Green et al.* (1957) to within 0.5 per cent.

For Stark broadening we use the theory of *Griem* (1960, 1964) for Hydrogen and ionized Helium as formulated by *Auer and Mihalas* (1972). This theory accounts for the perturbation of the atomic levels through electrons and ions. The ions are treated in a quasi static approximation: they produce instantaneously a mean electrical field of strength F in which the atom is immersed and a probability distribution is derived for the field strength. Electrons are treated with an impact theory: they are classical particles following classical paths; the atom is treated quantum mechanically and transitions within in the atom are taken into account.

A better theory for electrons, developed by *Vidal, Cooper and Smith* (1973) is used for the formal solution. In this theory, electrons are properly treated by accounting correctly for the transition between the impact and the quasi static approximations.

A.4. - Bound - Free Collisions

The bound - free collisional rates are calculated with the formula from *Mihalas* (1967), who used the experimental data of *Kieffer and Dunn* (1965) for the ground level, and a theoretical cross section from *Percival* (1966) for the excited levels. This allows Γ in the following expression to be fitted (see section II.4)

$$C_{ik} = \pi a_0^2 (8k/m\pi)^{1/2} n_e T^{1/2} e^{-h\nu_{ik}/kT} \Gamma(T) \quad (A.16)$$

where ν_{ik} is the frequency of the edge. The fit function $\Gamma(T)$ for all levels between $n = 1$ and $n = 10$, except for $n = 2$, is given by

$$\Gamma(T) = C_0 + C_1 \delta + C_2 \delta^2 + C_{-1} \delta^{-1} + C_{-2} \delta^{-2} \quad (A.17)$$

with $\delta = \log T$. For $n=2$ *Mihalas* gives

$$\Gamma_2(T) = C_0 + C_1 T + C_{-1} T^{-1} + C_{-2} T^{-2} \quad (A.18)$$

The values of the C - coefficients are shown in the Table A.4.

n	C_0	C_1	C_2	C_{-1}	C_{-2}
1	-.435	0.3	0.	0.	0.
2	.19987261 $\times 10^2$	-.58906298 $\times 10^{-4}$	0.	-.28185937 $\times 10^5$	.5444416 $\times 10^8$
3	.13935312 $\times 10^4$	-.16805859 $\times 10^3$	0.	-.2539 $\times 10^4$	0.
4	.20684609 $\times 10^4$	-.3341582 $\times 10^3$	0.	0.	-.76440625 $\times 10^4$
5	.32174844 $\times 10^4$	-.55882422 $\times 10^3$	0.	0.	-.686325 $\times 10^4$
6	.5759125 $\times 10^4$	-.15163125 $\times 10^4$	.8175 $\times 10^2$	0.	0.
7	.1461475 $\times 10^5$	-.4828375 $\times 10^4$	.39335938 $\times 10^3$	0.	0.
8	.2827925 $\times 10^5$	-.1017275 $\times 10^5$	.91967968 $\times 10^3$	0.	0.
9	.4679925 $\times 10^5$	-.176275 $\times 10^5$	.16742031 $\times 10^4$	0.	0.
10	-.74073 $\times 10^5$	.68599375 $\times 10^4$	0.	.201698 $\times 10^6$	0.

Table A.4 - Coefficients for (A.17) and (A.18) (Hydrogen)

For HeII, again an expression from *Percival* (1966) allows Γ in (A.16) to be fitted. *Mihalas and Stone* (1968) found that for levels 4 – 10 an expression similar to (A.17) may be used and for levels 1 – 3 one of the form (A.18). The coefficients are tabulated in Table A.5.

n	C_0	C_1	C_2	C_{-1}	C_{-2}
1	.073399521	1.4592763×10^{-7}	0.	- 237.75439	766212.99
2	1.7252867	$-2.0944117 \times 10^{-6}$	0.	- 2217.7891	5425487.9
3	8.6335087	$-2.7575544 \times 10^{-5}$	0.	- 5207.25	6639551.9
4	- 95.23828	62.656249	- 8.1454078	0.	0.
5	472.99219	- 74.144287	0.	0.	- 1869.6562
6	825.17186	- 134.23096	0.	0.	- 2739.4375
7	1181.3516	- 200.71191	0.	0.	- 2810.7812
8	1440.1016	- 259.75781	0.	0.	- 1283.5625
9	2492.125	- 624.84375	30.101562	0.	0.
10	4663.3129	- 1390.125	97.671874	0.	0.

Table A.5 – Coefficients for (A.17) and (A.18) (Helium II).

For the levels 11 – 20 *Seaton's* formula (1962) is used:

$$C_{ik} = 1.55 \times 10^{13} a_0 g n_e T^{-1/2} U_0 e^{-U_0} \quad (\text{A.19})$$

where a_0 is the photoionization cross section at threshold, $U_0 = h\nu_0/kT$ and the factor g is 0.1, 0.2 and 0.3 for $Z=0$, $Z=1$ and $Z \geq 2$, Z being the ionic charge.

The ionization rates for the ground level of HeI are calculated with the formula given by *Mihalas and Stone* (1968); this formula is an analytical fit by *Johnson* (1966) to experimental data from *Kieffer and Dunn* (1966)

$$C_{ik} = \pi a_0^2 (8k/m\pi)^{1/2} n_e T^{1/2} \sigma_0 \times \{U_0 E_1(U_0) - 0.728(U_0^2/U_1)E_1(U_1) - 0.189U_0^2 e^{-U_0} (2 + U_2)/U_2^3\} \quad (\text{A.20})$$

where $U_0 = \chi_n/kT$, $U_1 = U_0 + 0.27$, $U_2 = U_0 + 1.43$ and E_1 is the first exponential integral.

The rates with upper levels not explicitly considered in the calculations were added to the ionization rates in all cases.

A.5. – Bound – Bound Collisions

The bound – bound collisional rates of Hydrogen are calculated with the formula of *Peterson* (1969), who approximated the calculated values from *Burke, Ormonde and Whitaker* (1967) for $\Delta n = 1$ (n being the principal quantum number) by

$$C_{ij} = 4\pi a_0^2 (8k/m\pi)^{1/2} n_e T^{1/2} (E_H/h\nu_{ij})^2 U_0 f_{ij} \times \{ E_1(U_0) + 0.148 U_0 E_5(U_0) \} \quad (A.21)$$

where E_H is the ionization energy of Hydrogen, U_0 is $h\nu_{ij}/kT$ and E_1 and E_5 are again exponential integrals.

For $\Delta n > 1$ (A.21) is multiplied by a factor γ to bring it into agreement with the results of *Golden and Sampson* (1971):

$$\gamma = \beta + 2 (\alpha - \beta) / \Delta n \quad (A.22)$$

$$\text{with } \beta = 3 - 1.2/n \quad (A.23)$$

$$\alpha = 1.8 - 0.4/n^2 \quad (A.24)$$

n being the principal quantum number of the lower level i .

For HeII the excitation rates are calculated from the cross section proposed by *Hinnov* (1966). With it, *Mihalas and Stone* (1968) obtain

$$C_{ij} = \pi a_0^2 (8k/m\pi)^{1/2} n_e T^{1/2} (E_H/h\nu_{ij})^2 U_0 f_{ij} e \times \{ e^{-U_0} \ln 2 + U_0 E_1(U_0) \} \quad (A.25)$$

where E_H is again the ionization energy of Hydrogen and the transitions with $\Delta n > 1$ are scaled once more to reproduce the results from *Sampson and Golden* (1971). Hinnov's formula is based on semi - empirical arguments and agrees with measurements of the excitation rate of the $n = 2$ level and theoretical calculations of the $1s \leftrightarrow 2p$ transition of HeII.

For HeI, the excitation rates from the ground level to the levels with $n = 2$ are taken from the theoretical calculations of *Berrington et al.* (1982)

$$C'_{1j} = \{ b_0 + b_1 T^{-1/2} + b_2 T^{1/2} + b_3 T^{3/2} \} e^{-(E_{1j}/T)} \quad (A.26)$$

E_{1j} being the excitation energy expressed in Kelvin.

The coefficients b are given in Table A.6

	$1^1S \leftrightarrow 2^3S$	$1^1S \leftrightarrow 2^1S$	$1^1S \leftrightarrow 2^3P$	$1^1S \leftrightarrow 2^1P$
b_0	0.	4.32×10^{-9}	2.32×10^{-9}	0.
b_1	7.02×10^{-7}	0.	0.	0.
b_2	-4.37×10^{-13}	-3.21×10^{-12}	-1.85×10^{-12}	1.49×10^{-11}
b_3	0.	0.	0.	-6.78×10^{-18}

Table A.6 - Coefficients for (A.26)

For allowed transitions from the ground level to levels with $n > 2$ we use a formula taken from *Mihalas and Stone* (1968), which was obtained by fitting the experimental cross section of *Johnson* (1966):

$$C_{1j} = \pi a_0^2 (8k/m\pi)^{1/2} n_e T^{1/2} [4f_{1j} (E_H/E_0)^2] U_0 E_1(U_0) \quad (A.27)$$

From cross sections proposed by *Johnson* (1966), based on experimental data, *Mihalas and Stone* (1968) derived collisional values for forbidden transitions from the ground level to some upper levels

$$C_{1j} = \pi a_0^2 (8k/m\pi)^{1/2} n_e T^{1/2} \sigma_0 U_0$$

$$\times \{ a_0 E_1(U_0) + a_1 U_0 e^{-b_1 U_0} [b_1(U_0 + 1/c_1) + 2]/(U_0 + 1/c_1)^3$$

$$+ a_2 U_0 e^{-b_2 U_0} [b_2(U_0 + 1/c_2) + 2]/(U_0 + 1/c_2)^2 \} \quad (\text{A.28})$$

where $U_0 = E_{1j}/kT$, $\sigma_0 = a/n_{\text{eff}}^3$ (n_{eff} being the effective principal quantum number of level j) and the parameters a , a_0 , a_1 , b_1 , c_1 , a_2 , b_2 , c_2 for the transitions considered are listed in Table A.7.

Series	$a \times 10^{17}$ cm^2	a_0	a_1	b_1	c_1	a_2	b_2	c_2
$1^1 S \leftrightarrow n^1 S$	1.125	1.535	2.76	1.2	0.494	0.108	2.50	1.50
$1^1 S \leftrightarrow n^3 S$	1.240	0.230	17.8	1.0	0.080	5.400	1.00	0.35
$1^1 S \leftrightarrow n^3 P$	1.710	0.150	12.3	1.0	0.020	2.600	1.25	0.60
$1^1 S \leftrightarrow n^1 D$	1.02	1.240	1.68	1.2	0.906	0.181	2.70	1.45
$1^1 S \leftrightarrow n^3 D$	0.745	0.455	4.78	1.0	0.500	-0.075	1.50	2.00

Table A.7 – Coefficients for (A.28)

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Curriculum Vitae

I was born in Valencia (Spain) on February, the 26th 1959. My parents are Artemio Herrero – Campillo and Mercedes Davó – Pujadas. I attended the Colegio San Vicente Ferrer from January 1967 to June 1975 and the Academia García – Hernández, where I obtained my Bachiller Superior degree, from September 1975 to June 1976. In September 1976 I began my study in Physics at the University of Valencia, where I studied until June 1979. I then went to the University of La Laguna in September 1979, where I obtained my Licenciatura degree in June 1981, presenting my Tesina in December 1982. From December 1982 to October 1983 I worked at the Instituto de Astrofísica de Canarias and since November 1983 I have been working in the Institut für Astronomie und Astrophysik at the University in Munich.

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